I U C L I D

D a t a S e t

Existing Chemical	ID: 99-97-8
CAS No.	99-97-8
EINECS Name	N,N-dimethyl-p-toluidine
EINECS No.	202-805-4
Molecular Formula	C9H13N
Producer Related Part	
Company:	
Creation date:	21-OCT-1999
Substance Related Part	
Company:	
Creation date:	21-OCT-1999
Memo:	Bayer Corporation
Printing date:	29-OCT-2001
Revision date:	
Date of last Update:	29-OCT-2001
Number of Pages:	21
Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD and Company Information

Type: lead organisation
Name: American Chemistry Council (formerly Chemical Manufacturers Association), Monocyclic Aromatic Amines and Nitro Aromatics (MAANA) HPV Panel
Street: 1300 Wilson Boulevard
Town: 22209 Arlington, VA
Country: United States

21-AUG-2001

Type: cooperating company
Name: Albemarle Corpoiration
Country: United States

24-SEP-2001

Type: cooperating company
Name: Bayer Corporation
Country: United States

21-AUG-2001

Type: cooperating company
Name: Buffalo Color Corporation
Country: United States

21-AUG-2001

Type: cooperating company
Name: ChemFirst, Inc.
Country: United States

21-AUG-2001

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information
-

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms
-

1.3 Impurities
-

1.4 Additives
-

1.5 Quantity
-

1.6.1 Labelling
-

1.6.2 Classification
-

1.7 Use Pattern
-

1.7.1 Technology Production/Use
-

1.8 Occupational Exposure Limit Values
-

1.9 Source of Exposure
-

1.10.1 Recommendations/Precautionary Measures
-

1.10.2 Emergency Measures
-

1.11 Packaging
-

1.12 Possib. of Rendering Subst. Harmless
-

1.13 Statements Concerning Waste
-

1.14.1 Water Pollution
-

1.14.2 Major Accident Hazards
-

1.14.3 Air Pollution
-

1.15 Additional Remarks
-

1.16 Last Literature Search
-

1.17 Reviews
-

1.18 Listings e.g. Chemical Inventories
-

2.1 Melting Point

Value:	-6.6 degree C
Decomposition:	no
Sublimation:	no
Method:	other: (calculated) MPBPWIN v 1.30
Year:	1999
GLP:	no
Testsubstance:	other TS: molecular structure
Result:	Melting Point: -10.56 deg C (Adapted Joback Method) Melting Point: -2.61 deg C (Gold and Ogle Method) Mean Melt Pt : -6.59 deg C (Joback; Gold,Ogle Methods) Selected MP: -6.59 deg C (Mean Value)
Reliability:	(2) valid with restrictions Accepted calculation method
Flag:	Critical study for SIDS endpoint
21-AUG-2001	(1)

2.2 Boiling Point

Value:	211 degree C at 1013 hPa
Decomposition:	no
Method:	other:
GLP:	no data
Testsubstance:	other TS: N,N,4-trimethyl-benzenamine; purity not noted
Reliability:	(2) valid with restrictions Data from Handbook or collection of data
Flag:	Critical study for SIDS endpoint
21-AUG-2001	(2)

Value:	190.2 degree C
Method:	other: MPBPWIN (v1.31)
GLP:	no
Testsubstance:	other TS: molecular structure
Remark:	Adapted Stein and Brown Method
Reliability:	(2) valid with restrictions Accepted calculation method
Flag:	Critical study for SIDS endpoint
21-AUG-2001	(1)

2.3 Density

Type:	density
Value:	.9366 g/cm3 at 20 degree C
Method:	other
GLP:	no data
Testsubstance:	other TS: N,N,4-trimethyl-benzenamine; purity not noted
Reliability:	(2) valid with restrictions Data from Handbook or collection of data
Flag:	Critical study for SIDS endpoint
21-AUG-2001	(2)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: .78 hPa at 25 degree C
Method: other (calculated): MPBPWIN (v1.31)
GLP: no
Testsubstance: other TS: molecular structure
Result: Vapor Pressure Estimations (25 deg C):
(Using BP: 190.18 deg C (estimated))
(MP not used for liquids)
VP: 0.639 mm Hg (Antoine Method)
VP: 0.535 mm Hg (Modified Grain Method)
VP: 0.85 mm Hg (Mackay Method)

Selected VP: 0.587 mm Hg (Mean of Antoine & Grain methods)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
21-AUG-2001 (1)

Value: 1.33 hPa at 50 degree C
Method: other (measured)
GLP: no data
Testsubstance: other TS: N,N,4-trimethyl-benzenamine; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
21-AUG-2001 (3)

2.5 Partition Coefficient

log Pow: 2.81 at 25 degree C
Method: other (measured)
Year:
GLP: no data
Testsubstance: other TS: N,N-dimethyl-p-toluidine; purity not noted
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
21-AUG-2001 (4) (5)

log Pow: 2.718
Method: other (calculated): KOWWIN Program (v1.65)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
21-AUG-2001 (1)

log Pow: 2.61
Method:
Year:
Testsubstance: other TS: N,N-dimethyl-p-toluidine; purity not noted
Remark: Temperature: ambient
Method of equlibration: Shake-flask
Analytical method: absorption spectrophotometry
Aqueous phase: buffered solution of pH >7.0
Phase analyzed: aqueous
19-JUN-2001 (6) (7)

2.6.1 Water Solubility

Value: 455 mg/l
Qualitative: moderately soluble (100-1000 mg/L)
Method: other
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
24-SEP-2001 (8)

Value: 349.1 mg/l at 25 degree C
Qualitative: moderately soluble (100-1000 mg/L)
Method: other: (calculated) WSKOW (v1.36)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Remark: Log Kow (estimated) : 2.72
Log Kow (experimental): 2.81
Cas No: 000099-97-8
Name : Benzenamine, N,N,4-trimethyl-
Refer : Sangster 1993
Log Kow used by Water solubility estimates: 2.81

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW

Log Water Solubility (in moles/L) : -2.588
Water Solubility at 25 deg C (mg/L): 349.1
Reliability: (2) valid with restrictions
Accepted calculation method
21-AUG-2001 (1)

2.6.2 Surface Tension
-

2.7 Flash Point
-

2.8 Auto Flammability
-

2.9 Flammability
-

2.10 Explosive Properties
-

2.11 Oxidizing Properties
-

2.12 Additional Remarks
-

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1560000 molecule/cm3
Rate constant: .0000000002026656 cm3/(molecule * sec)
Degradation: 50 % after .6 hour(s)
Method: other (calculated): AOP Program v1.89
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
21-AUG-2001 (1)

3.1.2 Stability in Water

Type: abiotic
Method:
Year: GLP:
Test substance:
Remark: Hydrowin v1.67 cannot estimate a hydrolysis rate constant for this structure.
Flag: Critical study for SIDS endpoint
24-SEP-2001 (1)

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 106-49-0; 121-69-7.

3.1.3 Stability in Soil
-

3.2 Monitoring Data (Environment)
-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: air - biota - sediment(s) - soil - water
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: EPIWIN Level III Fugacity Model
Year: 1999
Result:

Media	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	0.156	1.27	1000	4.44e-012
Water	26.8	900	1000	1.48e-009
Soil	72.7	900	1000	6.68e-009
Sediment	0.329	3.6e+003	0	1.23e-009

Persistence Time: 525 hr
Reaction Time: 617 hr
Advection Time: 3.52e+003 hr
Percent Reacted: 85.1
Percent Advected: 14.9
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
21-AUG-2001 (1)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum:
Method: other: BIOWIN (v3.67) Program
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Result: Linear Model Prediction : Biodegrades Fast
Non-Linear Model Prediction: Does Not Biodegrade Fast
Ultimate Biodegradation Timeframe: Weeks-Months
Primary Biodegradation Timeframe: Days-Weeks
Flag: Critical study for SIDS endpoint
17-APR-2001 (1)

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 106-49-0; 108-44-1; 121-69-7; 103-69-5; 102-27-2; 91-66-7.

3.6 BOD5, COD or BOD5/COD Ratio
-

3.7 Bioaccumulation

Species: other
Exposure period:
Concentration:
BCF: 29.09
Elimination:
Method: other: BCF Program (v2.13)
Year: GLP: no
Test substance: other TS: molecular structure
Remark: Log Kow (estimated) : 2.72
Log Kow (experimental): 2.81
Log Kow used by BCF estimates: 2.81
Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70

Estimated Log BCF = 1.464 (BCF = 29.09)
Reliability: (2) valid with restrictions
Accepted calculation method
21-AUG-2001 (1)

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type:	flow through
Species:	Pimephales promelas (Fish, fresh water)
Exposure period:	96 hour(s)
Unit:	mg/l Analytical monitoring: yes
LC50:	52
EC50 :	52
Method:	EPA OPP 72-1
Year:	1980 GLP: no data
Test substance:	other TS: N,N-dimethyl-p-toluidine purchased from Aldrich Chemical Co., Milwaukee, WI; purity = 99%
Method:	pH was adjusted to approximate that of Lake Superior water (pH 7.8) with NaOH or HCL. Compound analyses were done by GLC: all exposure chambers at 0,24,48,72, and 96 hr. Fathead minnows used in this experiment were 35 days old and were cultured at US EPA Environmental Research Laboratory, Duluth, MN and University of Wisconsin - Superior campus. 20 fish/concentration and control. Behavior and toxic signs were noted at 4,24,48,72 and 96 hours.
Remark:	Affected fish lost schooling behavior and swam near the tank surface. They were hypoactive and under-reactive to external stimuli, and had increased respiration. Equilibrium loss was not observed prior to death. Alkalinity values increased with the exposure concentrations, due to a reaction between the titrant and the toxicant.

Test condition:	temperature = 25.7 degree C (+/-0.38);
	dissolved oxygen = 6.8 mg/l; pH =7.57;
	hardness = 38.9 mg/l CaCO3; tank volume = 1 liter;
	actual concentrations 11.1, 17.9, 26.2, 41.6, 65.1 mg/l.

Reliability:	(1) valid without restriction Guideline study
Flag:	Critical study for SIDS endpoint

24-SEP-2001 (9)

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: yes
LC50: 46
EC50 : 41.5
Method: EPA OPP 72-1
Year: 1980 GLP: no data
Test substance: other TS: N,N-dimethyl-p-toluidine purchased from Aldrich Chemical Co., Milwaukee, WI; purity = 99%
Method: pH was adjusted to approximate that of Lake Superior water (pH 7.8) with NaOH or HCL. Compound analyses were done by GLC: all exposure chambers at 0,24,48,72, and 96 hr.

Fathead minnows used in this experiment were 32 days old and were cultured at US EPA Environmental Research Laboratory, Duluth, MN and University of Wisconsin - Superior campus.

20 fish/concentration and control. Behavior and toxic signs were noted at 4,24,48,72 and 96 hours.
Remark: Affected fish lost schooling behavior and swam near the tank surface. They were hypoactive and under-reactive to external stimuli, and had increased respiration. Initial dissolved oxygen values were less than 60% of saturation. Equilibrium loss was not observed prior to death. The measured tank values were less than the nominal values. Alkalinity values increased with the exposure concentrations due to a reaction between the titrant and the toxicant.
Test condition: temperature = 24.9 degree C (+/-0.32);
dissolved oxygen = 5.0 mg/l; pH = 7.39;
hardness = 40.3 mg/l CaCO3; tank volume = 1 liter;
actual concentrations 11.8, 19.4, 30.9, 49.1, 71.3 mg/l.
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
24-SEP-2001 (10)

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: yes
LC50: 52.8
Method: other: American Society for Testing and Materials, 1980. Standard practice for conducting acute toxicity tests with fishes, macroinvertebrates, and amphibians. Annual Book of ASTM Standards. Philadelphia, PA, E729-80.
Year: 1980 GLP: no
Test substance: other TS: N,N-Dimethyl-p-toluidine (99-97-8) , purchased from Aldrich Chemical Company; chemical was of high purity
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
21-AUG-2001 (11)

Type: static
Species: Oryzias latipes (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: 20
Method: other: Japanese Industrial Standards Committee: "Testing Methods for Industrial Wastewater", JIS K0102, Japanese Industrial Standards Committee, p. 154 (1971)
Year: 1971 GLP: no data
Test substance: other TS: N,N-Dimethyl-p-toluidine (99-97-8) , purity: . not given
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
14-AUG-2000 (12)

Type: other: calculation
Species: other
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: 21.097
Method: other: (calculated) ECOSAR v0.99d
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
17-APR-2001 (1)

4.2 Acute Toxicity to Aquatic Invertebrates

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 23.758
Method: other: (calculated) ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
21-AUG-2001 (1)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: other algae: green algae
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 15.481
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
21-AUG-2001 (1)

4.4 Toxicity to Microorganisms e.g. Bacteria
-

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish
-

4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms
-

4.6.2 Toxicity to Terrestrial Plants
-

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species
-

4.7 Biological Effects Monitoring
-

4.8 Biotransformation and Kinetics
-

4.9 Additional Remarks
-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type:	LD50
Species:	rat
Strain:	Sprague-Dawley
Sex:	male/female
Number of Animals:	10
Vehicle:	other: neat
Value:	1650 mg/kg bw
Method:	OECD Guide-line 401 "Acute Oral Toxicity"
Year:	1987 GLP: yes
Test substance:	other TS: N,N-dimethyl-p-toluidine; purity = 99%
Remark:	No analysis of test material available; only method deviation - a constant dose volume was not used.
Reliability:	(1) valid without restriction GLP guideline study
Flag:	Critical study for SIDS endpoint

21-AUG-2001 (13)

5.1.2 Acute Inhalation Toxicity

Type:	LC50
Species:	rat
Strain:	Sprague-Dawley
Sex:	male/female
Number of Animals:	10
Vehicle:	other: neat
Exposure time:	4 hour(s)
Value:	1.4 mg/l
Method:	other: TSCA 40CFR 798.1150, July 1, 1991
Year:	1991 GLP: yes
Test substance:	other TS: N,N-dimethyl-p-toluidine; purity = 99%
Remark:	Submitted as TSCA substantial risk notice. No analysis of test material available; specification given
Reliability:	(1) valid without restriction GLP guideline study
Flag:	Critical study for SIDS endpoint

21-AUG-2001 (14)

5.1.3 Acute Dermal Toxicity

Type:	LD50
Species:	rabbit
Strain:	New Zealand white
Sex:	male/female
Number of Animals:	10
Vehicle:	other: neat
Value:	> 2000 mg/kg bw
Method:	OECD Guide-line 402 "Acute dermal Toxicity"
Year:	1987 GLP: yes
Test substance:	other TS: N,N-dimethyl-p-toluidine; purity = 99%
Remark:	No analysis of test material available; product specification given.
Reliability:	(1) valid without restriction GLP guideline study
Flag:	Critical study for SIDS endpoint

21-AUG-2001 (15)

5.1.4 Acute Toxicity, other Routes
-

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation
-

5.2.2 Eye Irritation
-

5.3 Sensitization
-

5.4 Repeated Dose Toxicity

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 106-49-0; 108-44-1; 121-69-7; 91-66-7.

5.5 Genetic Toxicity 'in Vitro'

Type: Bacterial reverse mutation assay
System of testing: Salmonella strains TA98, TA100, TA1537, TA1538
Concentration: 100, 333, 667, 1000, 3300, 5000 ug/plate
Cytotoxic Conc.: with metabolic activation: none
without metabolic activation: 1000 ug/plate
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year: 1983 GLP: yes
Test substance: other TS: N,N-dimethyl-p-toluidine; purity = 99%
Remark: No analysis of test material; specification given . Only deviation from the testing guideline was the lack of a confirmatory assay.
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
21-AUG-2001 (16)

Type: Cytogenetic assay
System of testing: Chinese hamster V79 cells
Concentration: 0, 0.3, 0.9, 1.2 mM
Cytotoxic Conc.: > 10% survival at 1.2mM as estimated by colony formation
Metabolic activation: without
Result: positive
Method: other: S. Bonatti et al, Mutat. Res. 116, 149-154 (1983)
Year: GLP: no data
Test substance: other TS: N,N-dimethyl-p-toluidine; purity not noted
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
21-AUG-2001 (17)

Type: Bacterial reverse mutation assay
System of testing: Salmonella strains TA97, TA98, TA100
Concentration: 0, 1, 2.5, 5, 10, 40, 70, 100 ug/plate
Cytotoxic Conc.: 100 ug/plate
Metabolic activation: with and without
Result: negative
Method: other: Maron, D.M., and Ames, B.N., Mutat. Res. 113, 173-215
Year: 1983 GLP: no data
Test substance: other TS: N,N-dimethyl-p-toluidine; purity = 99%
Reliability: (2) valid with restrictions
24-SEP-2001 (17)

5.6 Genetic Toxicity 'in Vivo'

Type: other: Alkaline elution assay
Species: mouse Sex:
Strain: Balb/c
Route of admin.: i.p.
Exposure period: single dose
Doses: 0, 1, or 2 mmol/kg (0, 135, 270 mg/kg)
Result: negative
Method: other: Parodi, S. et al, Mutat. Res. 54, 39-46 (1978)
Year: 1978 GLP: no data
Test substance: other TS: N,N-dimethyl-p-touludine; purity = 99%
Remark: The author mentions that an increase of 3X controls is usually considered positive.
Result:

dose mmol/kg	2 hr	24 hr
0	2.15	2.06
1	2.05	3.43
2	2.39	----

28-SEP-2001 (17)

Type: other: Alkaline elution assay
Species: rat Sex:
Strain: Sprague-Dawley
Route of admin.: oral unspecified
Exposure period: single dose
Doses: 0 and 8 mmol/kg (0 and 1080 mg/kg)
Result: ambiguous
Method: other: Parodi, S. et al, Mutat. Res. 54, 39-46 (1978)
Year: 1978 GLP: no data
Test substance: other TS: N,N-dimethyl-p-touludine; purity = 99%
Remark: DNA fragmentation increased in liver cells to about 2.4 X control at one dose only. The author mentions that an increase of 3X controls is usually considered positive. That is why he considers this a weak positive.
Result: weak positive

dose mmol/kg	6 hr	24 hr
0	1.36	1.48
8	3.22**	1.85

DNA fragmentation increased in liver cells to about 2.4 X control at one dose only.

28-SEP-2001 (17)

Type: other: Alkaline elution assay
Species: rat Sex:
Strain: Sprague-Dawley
Route of admin.: i.p.
Exposure period: single dose
Doses: 0, 4, and 8 mmol/kg (0, 540, and 1080 mg/kg)
Result: ambiguous
Method: other: Parodi, S. et al, Mutat. Res. 54, 39-46 (1978)
Year: 1978 GLP: no data
Test substance: other TS: N,N-dimethyl-p-touludine; purity = 99%
Remark: DNA fragmentation increased in liver cells to about 2X control at one dose only. The author mentions that an increase of 3X controls is usually considered positive. That is why he considers this a weak positive.
Result: weak positive

dose mmol/kg	2 hr	24 hr
0	1.63	1.99
4	3.14	2.06
8	3.23*	----

DNA fragmentation increased in liver cells to about 2X control at one dose only.

28-SEP-2001 (17)

5.7 Carcinogenicity

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5.8 Toxicity to Reproduction

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 106-49-0; 108-44-1; 121-69-7.

5.9 Developmental Toxicity/Teratogenicity

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 121-69-7; 91-66-7.

5.10 Other Relevant Information

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5.11 Experience with Human Exposure

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(1) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510.

(2) CRC Handbook of Chemistry and Physics. 80th ed. (1999) David
R. Lide, ed. CRC Press, New York. p. 3-26, No. 862.

(3) CRC Handbook of Chemistry and Physics. 55th ed, (1974) p. D-180.

(4) Sangster, J. (1989). J. Phys. Chem. Ref. Data 18:1205.

(5) Schultz OE, Jung C. Moeller KE. (1970) Z. Naturforscher B. 25:1024

(6) Norrington FE, Hyde RM, Williams SG, Wootton R. 1975. J. Med Chem. 18:604.

(7) Sangster, J. (1989). J. Phys. Chem. Ref. Data 18:1205.

(8) Verschueren, K. (2001) Handbook of Environmemtal Data on Organic Chemicals. 4th edition. Vol. 1 p. 944

(9) Geiger, D.L. et al. (1986) "Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas), Vol. 3, Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI, p.221-2 (test 1).

(10) Geiger, D.L. et al. (1986) "Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales promelas), Vol. 3, Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI, p.223-224 (test 2).

(11) Broderius, S. and Kahl, M. (1985) Aquat. Toxicol. 6: 307-322.

(12) Tonogai, Y. et al. (1982) J. Toxicol. Sci. 7, 193-203.

(13) ChemFirst Study No. 3888-91-0105-TX-001

(14) ChemFirst Study No. L08413

(15) ChemFirst Study No. 3888-91-0106-TX-001

(16) ChemFirst Study No. 14506-0-401

(17) Taningher, M. et al, (1993) Environ. Mol. Mutagen. 21: 349-356.

7.1 End Point Summary

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7.2 Hazard Summary

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7.3 Risk Assessment

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D a t a S e t

Existing Chemical	Substance ID: 95-53-4
CAS No.	95-53-4
EINECS Name	o-toluidine
EINECS No.	202-429-0
Molecular Weight	107.2
Molecular Formula	C7H9N

2. Physico-chemical Data

2.1 Melting Point

Value:	-16.3°C
Reference:	CRC Handbook of Chemistry and Physics, 80th ed, p 3-24 (1999).

2.2 Boiling Point

Value:	200.3°C
Reliability:	(1) valid without restriction
Flag:	**robust summary**
Reference:	CRC Handbook of Chemistry and Physics, 80th ed, p 3-24 (1999).

2.3 Density

Type:	relative density
Value:	.9984 at 20°C
Reliability:	(1) valid without restriction
Flag:	**robust summary**
Reference:	CRC Handbook of Chemistry and Physics, 80th ed, p 3-24 (1999).

2.4 Vapour Pressure

Value:	0.26 mm
Temperature:	25°C
Method:	calculated[ ]; measured [x]
GLP:	Yes[ ] No[ ] ?[ ]
Remarks:	
Reference:	Danner, R.P., Physical and Thermodynamic Properties of Pure Chemicals, Design Inst. Phys. Prop. Data. Amer. Inst. Chem. Eng. NY; NY: Hemisphere Pub. Corp. Vol. 4 (1989).

2.5 Partition Coefficient

log Pow: 1.4 at 24.5 °C
Method: Directive 84/449/EEC, A.8 "Partition coefficient"
Year:
GLP: yes
Reference: BASF AG (1987): Unvergeffentlichte Untersuchung der Abt Analytik (Bericht-Nr. 87.19.10).

2.6.1 Water Solubility

Value: 8 g/l at 20°C
pH: 7.5 at 8 g/l and 20°C
Reference: BASF AG (1992): Sicherheitdatenblatt ortho-Toluidin (Aug. 1992).

3.1.2 Stability in Water
Type: Abiotic (hydrolysis) [x]; biotic (sewdiment) [ ]
Degradation: 4.0±5.6% at pH approx. 6.4 at 30°C after 48 hours.
Method: Schultz, T.W. et al, Bull. Environ. Toxicol. Chem. 42, 192-198 (1989);Yoshioka, Y. et al, Sci. Total Environ. 43, 149-157 (1985).
GLP: Yes[ ] No[x] ?[ ]
Remarks: Concentration tested was 380 mg/L.
Reference: Arnold, L.M. et al, Chemosphere 21 (1-2), 183-191 (1990).

3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge
Degradation: 88 - 90 % after 28 day
Method: OECD Guide-line 301 A (old version) "Ready biodegradabiltiy: Modified AFNOR Test"
Year: GLP: no
Test substance: no data
Remark: DOC Analysis:
7 day (74 - 89 %)
14 day (73 - >90 %)
Reference: Brown D., and Laboureur, P., Chemosphere 12(3), 405-414 (1983).

Type: aerobic
Inoculum: activated sludge
Degradation: > 90 % after 28 day
Method: OECD Guide-line 301 A (old version) "Ready Biodegradabiltiy: Modified AFNOR Test"
Year: GLP: no
Test substance: no data
Remark: Specific (gas chromatography) analysis:
7 day (>90 %)
14 day (>90 %)
Reference: Brown D., and Laboureur, P., Chemosphere 12(3), 405-414 (1983).

Type: aerobic
Inoculum: activated sludge

Degradation: > 90 % after 28 day
Method: OECD Guide-line 301 E "Ready biodegradability: Modified OECD Screening Test"
Year: GLP: no
Test substance: no data
Remark: DOC Analysis:
7 day (57 - >90 %)
14 day (>90 %)
Flag: **robust summary**
Reference: Brown D., and Laboureur, P., Chemosphere 12(3), 405-414 (1983).

Type: aerobic
Inoculum: activated sludge
Degradation: > 90 % after 28 day
Method: OECD Guide-line 301 E "Ready biodegradability: Modified OECD Screening Test"
Year: GLP: no
Test substance: no data
Remark: Specific (gas chromatography) analysis:
7 day (57 - >90 %)
14 day (>90 %)
Reference: Brown D., and Laboureur, P., Chemosphere 12(3), 405-414 (1983).

3.7 Bioaccumulation

Species: Crassostrea gigas, Pacific oyster; static
Exposure period: 24 hour
Concentration: 5 mg/l
BCF: 4.6
GLP: No data
Reference: Knezovich, J.P. and Crosby, D.G., Environ. Toxicol. Chem. 4(4), 435-446 (1985).

Species: Mytilus edulis, Common bay mussel; static
Exposure period: 24 hour
Concentration: 5 mg/l
BCF: 4.2
GLP: No data
Reference: Knezovich, J.P. and Crosby, D.G., Environ. Toxicol. Chem. 4(4), 435-446 (1985).

4.0 Ecotoxicity

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no data
EC50: .52
Method: other: NEN 6501, 1980
Year: GLP: no data
Test substance: purity > 99.5 %
Source: Bayer AG Leverkusen
Reliability: (2) valid with restrictions
Flag: **robust summary**

Reference: Maas-Diepeveen, J.L. and van Leeuwen, C.J.: Aquatic toxicity of aromatic nitro compounds and anilines to serveral freshwater species. Laboratory for Ecotoxicology, Institute for Inland Water Management and Waste Water Treatment,Ministry of Transport and Public Works, P.O.Box 17, 8200 AA Lelystad, The Netherlands, DBW/RIZA Report 86-42, tvl1296/84

Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring: no
EC0: 1.6 - 5
EC50: 9 - 50
EC100: 100
Method: other: Daphnia Immobilization test; s. Authors of this publication
Year: GLP: no
Test substance: no data
Source: Bayer AG Leverkusen
Reference: Bringmann, G., and Kuehn, R., Z. Wasser Abwasser Forsch. 15(1), 1-6 (1982).

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Chlorella pyrenoidosa (Algae)
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 55
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984 GLP: no data
Test substance: other TS: purity: > 99.5%
Source: Bayer AG Leverkusen
Reliability: (1) valid without restriction
Flag: **robust summary**
Reference: Maas-Diepeveen, J.L. and van Leeuwen, C.J.: Aquatic toxicity of aromatic nitro compounds and anilines to several freshwater species. Laboratory for Ecotoxicology, Institute for Inland Water Management and Waste Water Treatment,Ministry of Transport and Public Works, P.O.Box 17, 8200 AA Lelystad, The Netherlands, DBW/RIZA Report 86-42, tvl1296/84

Species: Scenedesmus subspicatus (Algae)
Endpoint: biomass
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 3.9
Method: other: DIN 38412 part 9
Year: GLP: no
Test substance:
Reference: Kuehn, R. and Pattard, M., Wat. Res. 24 (1), 31-38 (1990)

5. Toxicity

Species:	rat	Sex: male
Strain:	Fischer 344	
Route of admin.:	oral gavage; no vehicle	
Exposure period:	5, 10, or 20 Days	
Frequency of treatment:	daily	
Post. obs. period:	none	
Doses:	225 mg/kg body weight per day	
Control Group:	yes; sham dosed	
Method:	Described in the publication	
Year:		GLP: no data
Test substance:	99.3% purity	
Result:	Deaths, decreased body weights(5 and 10 days) and increased spleen weights; transient cyanosis after dosing; rough hair coat; splenic congestion, increased hematopoiesis and hemosiderosis, and bone marrow hyperplasia.	
Comments:	Blood changes were consistent with enhanced erythrocyte destruction.	
Reference:	Short, C.R. et al, Fundam. Appl. Toxicol. 3, 285-292 (1983).	

Species:	rat	Sex: male and female
Strain:	F344/N	
Route of admin.:	dietary	
Exposure period:	7 weeks	
Frequency of treatment:	daily	
Post. obs. period:	1 week	
Doses:	1000, 2000, 3000, 4000, 6000, 6200, 12,500, 25,000, and 50,000 ppm in diet	
Control Group:	basal diet only	
Method:	no information	
Year:		GLP: no data
Test substance:	Hydrochloride salt, purity reported as >99%	
Result:	Deaths at 50,000 ppm; renal and splenic pigmentation at 12,500 ppm; greater than 10% reduction in body weights compared to controls at 12,500 ppm and higher levels.	
Comments:	Purpose was to select doses for carcinogenicity study.	
Reference:	NCI Technical Report Series No. 153, Bioassay of o-toluidine hydrochloride for possible carcinogenicity, NCI-CG-TR-153, 1979.	

Species:	mouse	Sex: male and female
Strain:	B6C3F1	
Route of admin.:	dietary	
Exposure period:	7 weeks	
Frequency of treatment:	daily	
Post. obs. period:	1 week	

Doses: 3100, 6200, 8000, 10,000, 12,500, 20,000, 25,000, and 50,000 ppm in diet
Control Group: basal diet only
Method: no information
Year: GLP: no data
Test substance: Hydrochloride salt, purity reported as >99%
Result: Pigment deposition in the spleen and smaller amounts in the kidneys and liver at 50,000 ppm; greater than 10% reduction in body weights compared to controls at all dietary levels.
Comments: Purpose was to select doses for carcinogenicity study.
Reference: NCI Technical Report Series No. 153, Bioassay of o-toluidine hydrochloride for possible carcinogenicity, NCI-CG-TR-153, 1979.

Species: rat Sex: male
Strain: F344/N
Route of admin.: dietary
Exposure period: 13 or 26 weeks
Frequency of treatment: daily
Post. obs. period: 13 weeks, after 13 weeks of dietary exposure
Doses: 5000 ppm in diet
Control Group: basal diet only
Method: no information
Year: GLP: no data
Test substance: Hydrochloride salt, purity reported as 100%
Remarks: 20 rats/group; 80 rats total. 20 had altered gut flora.
Result: Decreased weight gain; increased hematopoiesis, hemosiderosis, congestion, and fibrosis in the spleen; increased spleen weights; minimal hemosiderosis in the liver; hyperplasia of the bladder epithelium; mesothelial hyperplasia and mesothelioma.
Comments:
Reference: NTP Toxicity Report Series No. 44, NTP technical report on comparative toxicity and carcinogenicity studies of o-nitrotoluene and o-toluidine hydrochloride, NIH Publication 96-3936 (March 1996).

5.7 Carcinogenicity

Species: rat Sex: male
Strain: Charles River
Route of admin.: dietary
Exposure period: 18 months
Frequency of treatment: daily
Post. obs. period: 6 months
Doses: 0, 8000, 16000 ppm for 3 months; then 4000 and 8000 ppm for 15 months
Control Group: basal diet

Method: no information
Year: GLP: no data
Test substance: Hydrochloride salt; 97-99% purity
Remark: 25 rats per group

Result: Weight gain decreased by at least 10% at 16000 ppm at 3 months; dose-related increased incidence of subcutaneous fibromas and fibrosarcomas, transitional cell carcinomas of the bladder, and multiple tumors (pituitary and adrenal).
Reference: Weisburger, E.K. et al, J. Environ. Pathol. Toxicol. 2, 325-356 (1978).

Species: mouse Sex: male and female
Strain: HaM/ICR
Route of admin.: dietary
Exposure period: 18 months
Frequency of treatment: daily
Post. obs. period: 6 months
Doses: 0, 16,000, 32,000 ppm for 3 months; then 8000 and 16000 ppm for 15 months
Control Group: basal diet
Method: no information
Year: GLP: no data
Test substance: Hydrochloride salt; 97-99% purity
Remark: 25 mice per group

Result: Weight gain decreased by at least 10% at 32000 ppm at 3 months; dose-related increased incidence of hemangiomas and hemangiosarcomas.
Reference: Weisburger, E.K. et al, J. Environ. Pathol. Toxicol. 2, 325-356 (1978).

Species: rat Sex: male and female
Strain: F344
Route of admin.: dietary
Exposure period: up to 104 weeks
Frequency of treatment: daily
Post. obs. period: none
Doses: 0, 3000, 6000 ppm
Control Group: basal diet
Method: no information
Year: GLP: no data
Test substance: Hydrochloride salt, purity reported as >99%
Remark: 50 animals/sex/group; Control group: 20 animals/sex.
Result: Dose-related increased deaths and decreased body weight gains, increased incidence of fibrosarcomas, angiosarcomas, and osteosarcomas in the spleen and other organs, mesotheliomas of the abdominal cavity or scrotum in males, and transitional cell carcinomas of the urinary bladder in females. Also increased fibromas in subcutaneous tissue in males and

fibroadenomas or adenomas of the mammary gland in females.

Reference: NCI Technical Report Series No. 153, Bioassay of o-toluidine hydrochloride for possible carcinogenicity, NCI-CG-TR-153, 1979.

Species: mouse Sex: male and female
Strain: B6C3F1
Route of admin.: dietary
Exposure period: up to 104 weeks
Frequency of treatment: daily
Post. obs. period: none
Doses: 0, 1000, 3000 ppm
Control Group: basal diet
Method: no information
Year: GLP: no data
Test substance: Hydrochloride salt, purity reported as >99%
Remark: 50 animals/sex/group; Control group: 20 animals/sex.
Result: Dose-related decreased body weight gains, hemangiosarcomas at various sites in males, and hepatocellular carcinomas or adenomas in females.
Reference: NCI Technical Report Series No. 153, Bioassay of o-toluidine hydrochloride for possible carcinogenicity, NCI-CG-TR-153, 1979.

5.5 Genetic Toxicity 'in Vitro'

Type: Cytogenetic assay
System of testing: Chinese hamster ovary (CHO) cells
Concentration: 250, 500 ug/ml
Metabolic activation: with and without
Result: Positive
Method: Galloway, S.M. et al. (1985): Environ. Mutagen. 7(1), 1-51
Year: GLP: no data
Test substance: Purity was >99%
References: Dean, B.J.(1985): Prog. Mut. Res 5, 69-83; Gulati, B.K. et al. (1985): Prog. Mut. Res. 5, 413-426

Type: Cytogenetic assay
System of testing: Chinese hamster lung (CHL) fibroblast cells
Concentration: 1000-1500 ug/ml
Metabolic activation: with and without
Result: Positive
Method: Given in publication
Year: GLP: no data
Test substance: Purity was >99%

References: Dean, B.J.(1985): Prog. Mut. Res. 5, 69-83; Ishidate,Jr., M., and Sofuni, T., (1985): Prog. Mut. Res. 5, 427-432

Type: Cytogenetic assay
System of testing: Chinese hamster ovary (CHO) cells
Concentration: up to 2142 ug/ml
Metabolic activation: with and without
Result: Negative
Method: Given in publication
Year: GLP: no data
Test substance: Purity was >99%
References: Dean, B.J.(1985): Prog. Mut. Res. 5, 69-83; Natarajan, A.T. et al. (1985): Prog. Mut.Res. 5, 433-437

Type: Cytogenetic assay
System of testing: Chinese hamster ovary (CHO) cells
Concentration: up to 900 ug/ml
Metabolic activation: with and without
Result: Negative
Method: Given in publication
Year: GLP: no data
Test substance: Purity was >99%
Source: Bayer AG Leverkusen
References: Dean, B.J.(1985): Prog. Mut. Res. 5, 69-83; Palitti, F. et al. (195): Prog. Mut. Res. 5, 443-450

Type: Cytogenetic assay
System of testing: Chinese hamster primary liver (CH1-L) cells
Concentration: up to 120 ug/ml
Metabolic activation: intrinsic; none added
Result: Negative
Method: other
Year: GLP: no data
Test substance: Purity was >99%
Remark: mitosis and mitotic spindle assay
References: Parry J.M. et al. (1984): Altern. Lab. Anim. 11, 117-128; Parry, J.M. (1985): Prog. Mut. Res. 5, 479-485

Type: Cytogenetic assay
System of testing: RL 4 (rat liver)
Concentration: 700 ug/ml was lowest effective dose
Metabolic activation: intrinsic; none added
Result: Positive
Method: other
Year: GLP: no data
Test substance: Purity was >99%

References: Priston, R.A.J., and Dean, B.J.(1985): Prog. Mutat. Res. 5, 387-395

Type: Cytogenetic assay
System of testing: Chinese hamster primary liver (CH1-L) cells
Concentration: 12 ug/ml was lowest effective dose
Metabolic activation: intrinsic; none added
Result: Positive
Method: no information
Year: GLP: no data
Test substance: Purity was >99%
References: Danford N.(1985): Prog. Mutat. Res. 5, 397-411; Danford, N.(1991): Mutat. Res. 258, 207-236

Type: Cytogenetic assay
System of testing: Chinese hamster lung (CHL) cells
Concentration: 1000 ug/ml was lowest effective dose
Metabolic activation: with and without
Result: Positive with activation; negative without activation at 1500 ug/ml
Method: no information
Year: GLP: no data
Test substance: no data
References: Ishidate Jr.,M., et al. (1988): Mutat. Res. 195, 151-213

Type: Cytogenetic assay
System of testing: Chinese hamster lung (CHL) cells
Concentration: 500 ug/ml was lowest effective dose with activation; 1000 ug/ml was negative without activation
Metabolic activation: with and without
Result: Positive with activation
Method: no information
Year: GLP: no data
Test substance: no data
References: Ishidate Jr.,M., et al. (1988): Mutat. Res. 195, 151-213

Type: Cell transformation
System of testing: Baby hamster kidney cells (BHK 21 C13/HRC 1)
Concentration: 606 ug/ml was lowest effective dose without activation; 362 ug/ml was lowest effective dose with activation
Metabolic activation: with and without
Result: Positive with and without activation
Method: other
Year: GLP: no data
Test substance: no data
Flag: **robust summary**

References: Brookes, P., and Preston, R.J.(1981): Prog. Mut. Res. 1, 77-85; Daniel,M.R., and Dehnel, J.M.(1981): Prog. Mut. Res. 1, 626-637

Type: Cell transformation
System of testing: Baby hamster kidney cells; BHK 21/clone
Concentration: 250 ug/ml with activation was lowest effective dose
Metabolic activation: with
Result: Positive
Method: other
Year: GLP: no data
Test substance: no data
References: Brooks, T.M., et al. (1981): Prog. Mut. Res. 1, 77-85; Styles, J.A. (1981): Prog. Mut. Res. 1, 638-646

Type: Cell transformation
System of testing: Syrian hamster embryo cells
Concentration: 1 ug/ml was lowest effective dose
Metabolic activation: without
Result: Positive
Method: other
Year: GLP: no data
Test substance: Purity was >99%
References: Barrett, J.C., and Lamb, P.W.(1985): Prog. Mut. Res. 5, 623-628

Type: Cell transformation assay
System of testing: Syrian hamster embryo (SHE cells)
Concentration: 100 ug/ml was lowest effective dose
Metabolic activation: none
Result: Positive
Method: no information
Year: GLP: no data
Test substance: Purity was >99%
References: Sanner, T., and Rivedal, E.; cited in: Ashby et al. (eds.) (1985): Prog. Mutat. Res. 5, 665-671; cited in: Danford (1991): Mutat. Res. 258, 207-236

Type: Cell transformation assay
System of testing: Syrian hamster embryo (SHE) cells
Concentration: 965 ug/ml was lowest effective dose
Metabolic activation: none
Result: Positive
Method: Adenovirus (SA7) transformation assay as prescribed by Casto, B.C. (1973): Progr. Esp. Tumor Res. 18, 166-198
Year: GLP: no data
Test substance: Purity was >99%

Reference: Hatch, G.G. and Anderson, T.M. (1985): Prog. Mutat. Res. 5, 629-638

Type: Cell transformation assay
System of testing: Balb/c-3T3
Concentration: 330 ug/ml was highest ineffective dose without activation; 150 ug/ml was lowest effective dose with activation
Metabolic activation: primary rat liver cells co-cultivation
Result: Positive with added rat liver cells
Method: Kakunaga, T. (1973): Int. J. Cancer 12, 463-473
Year: GLP: no data
Test substance: no data
Reference: Matthews, E.J. et al (1985): in F.J. de Serres and J. Ashby (Eds.), Evaluation of Short-Term Tests for Carcinogens, Progr. Mutat. Res.5, 639-650

Type: Cell Transformation Assay
System of testing: AKR leukemia virus infected NIH Swiss mouse embryo (AKH-NIH-ME) cells
Concentration: 1 and 10 ug/ml
Metabolic activation: none
Result: Weak positive
Method: other
Year: GLP: no data
Test substance: no data
References: Heidelberger, C. et al. (1983): Mutat. Res. 114, 283-285; Rhim, J.S. et al. (1974): J. Natl. Cancer Inst. 52, 1167-1173.

Type: other: cell transformation assay
System of testing: embryonic mouse fibroblasts (C3H/10T1/2 Clone 8)
Concentration: 600 ug/ml was lowest effective dose with activation
Metabolic activation: with and without
Result: Positive
Method: Reznikoff, C.A. et al. (1973): Cancer Res. 33, 3231-3238
Year: GLP: no data
Test substance: Purity was >99%
References: Lawrence, N., and McGregor, D.B. (1985): Prog. Mut. Res. 5, 651-658; Nesnow, S. et al. (1984): Health Effects Research Lab. USEPA, PB84-167501; Nesnow, S. et al. (1985): Prog. Mut. Res. 5, 659-664

Type: other: cell transformation assay
System of testing: Chinese hamster ovary (CHO) cells
Concentration: 500 ug/ml was the highest ineffective dose
Metabolic activation: with and without
Result: Negative

Method: Pienta, R.J. et al (1977): Int. J. Cancer 19, 642-655
Year: GLP: no data
Test substance: Purity was >99%
Reference: Garner, R.C.(1985): Prog. Mut. Res. 5, 85-94; Zdzienicka, M.C. et al. (1985): Prog. Mut. Res. 5, 685-688

5.6 Genetic Toxicity 'in Vivo'

Type: Cytogenetic assay
Species: mouse Sex: male
Strain: CD-1
Route of admin.: intraperitoneal
Exposure period: One to 4 treatments at 24 hr intervals
Doses: 100, 200, 400, 800, and 1000 mg/kg bw
Method: no data; method described in publication
Year: GLP: no data
Remarks: Six independent assays were done
Test substance: Purity was 99%
Result: Negative
Reference: Morita, T. et al (1997): Mutat. Res. 389, 3-122

Type: Cytogenetic assay
Species: mouse Sex: male
Strain: B6C3F1
Route of admin.: intraperitoneal
Exposure period: single administration
Doses: 150, 300, 600 mg/kg bw
Method: MacGregor, J.T. et al (1987): Mutat. Res. 189, 103-112
Year: GLP: no data
Test substance: Hydrochloride salt, obtained from NTP
Result: negative
Reference: McFee, A.F. et al. (1989): Environ. Molec. Mutagen. 14, 207-220

Type: Cytogenetic assay
Species: hamster Sex: no data
Strain: no data
Route of admin.: oral unspecified
Exposure period:
Doses: 100 - 300 mg/kg body weight
Method: no information
Year: GLP: no data
Test substance: no data
Result: Negative
Flag: **robust summary**
Reference: MAK-Begruendung (1986)

Type: Cytogenetic assay
Species: mouse Sex: no data
Strain: no data
Route of admin.: intraperitoneal
Exposure period:
Doses: 45 mg/kg body weight
Method: no information
Year: GLP: no data

Test substance: no data
Result: Positive
Reference: MAK-Begruendung (1986)

Type: Micronucleus assay
Species: mouse Sex: male
Strain: B6C3F1
Route of admin.: intraperitoneal
Exposure period: single administration
Doses: 75, 150, 300 mg/kg bw
Method: MacGregor, J.T. et al (1987): Mutat. Res. 189, 103-112
Year: GLP: no data
Test substance: Hydrochloride salt, obtained from NTP
Result: negative
Reference: McFee, A.F., et al. (1989): Environ. Molec. Mutagen. 14, 207-220

Type: Micronucleus assay
Species: mouse Sex: no data
Strain: B6C3F1
Route of admin.: intraperitoneal
Exposure period:
Doses: 40, 80, 160, 169, 270, 338 ul/kg body weight
Method: no information
Year: GLP: no data
Result: Negative
Test substance: Hydrochloride salt
Reference: Purchase, I.F.H.(1981): Prog. Mutat. Res. 1, 86-95; Salamone, M.F.et al. (1981): Prog. Mutat. Res. (De Serres, Ashby,eds.) 1, 686-697; cited in Danford, N.,(1991): Mutat. Res. 258, 207-236; Tsuchimoto, T. and Matter, B.E. (1981): Prog. Mutat. Res. (De Serres,Ashby, eds.) 1, 705-711; cited in Danford, N.,(1991): Mutat. Res. 258, 207-236

Type: Mouse Sperm Abnormality Test
Species: mouse Sex: male
Strain: CBAXBALB/C F1 hybrids
Route of admin.: intraperitoneal
Exposure period: 5 Days
Doses: 0.05 - 0.5 mg/kg body weight
Method: no information
Year: GLP: no data
Test substance: Hydrochloride salt
Result: Negative
Reference: Purchase, I.F.H.(1981): Prog. Mut. Res. 1, 86-95; Topham, J.C.(1980): Mutat. Res. 74, 379-387;Topham, J.C.(1981): Prog. Mut. Res. 1, 718-720

5.8 Toxicity to Reproduction

Species: rat Sex: male/female
Strain: no data
Route of admin.: dermal
Exposure period: 4 months
Frequency of

treatment:	4 hr/day
Post. obs. period:	Treated rats of both sexes were mated with untreated at 4 months and the offspring maintained until 2 month of age
Doses:	8, 80 mg/kg body weight
Control Group:	yes
Method:	no information
Year:	GLP: no data
Test substance:	no data
Remark:	Test substance was applied to 2/3 of the tail skin; 15 rats/sex/group. Some animals were killed at 4 months and examined for pathology while the others were mated and the offspring maintained until 2 months of age. There was no further treatment of parental animals during mating, gestation, and lactation.
Result:	There was no change in testes or ovary weights, and no change in nucleic acids in the ovaries. The amount of testicular RNA in homogenates was significantly decreased at 80 mg/kg. The number of corpora lutea increased at 8 mg/kg, while the number of primordial follicles decreased at 80 mg/kg. Estrus length was also increased at 80 mg/kg compared to controls. There was a stimulation of spermatogenesis at both dose levels; the effect was greater at the lower dose. Sertoli cells increased in size and functioning. There were no pathological, structural, or functional changes in germ cells. Spermatogenesis and testicular morphology returned to normal during the post-exposure period. Treatment did not affect fertility, litter size, offspring body weights, or survival of offspring. Litters from females treated with 80 mg/kg were weaker and slower to gain weight compared to controls. This retardation of development persisted during the first month of life and was most marked in female pups. The offspring of females treated with 8 mg/kg had decreased body weight gain at 1.5 months of age. These differences were no longer significant at 2 month of age. The offspring of treated males were not affected. There were no changes in the blood, reproductive organ nucleic acids, or blood serum of pups. Female pups from treated females had increased mean kidney weights at both doses, and increased mean ovary and heart weights at 80 mg/kg only. Male pups from treated females given 80 mg/kg had decreased mean spleen and lung weights. Female pups from high dose treated males had increased mean lung and adrenal weights, while male pups from these males had decreased mean liver and spleen weights. The authors conclude that the effective dose for toxicity to the reproductive organs is the same as that for general toxicity via dermal exposure, and is equal to 80 mg/kg.
Reference:	Malysheva,M.V. et al. (1983): Gig. Tr. Prof. Zabol. 9, 47-49

I U C L I D

D a t a S e t

Existing Chemical	ID: 91-66-7
CAS No.	91-66-7
EINECS Name	N,N-diethylaniline
EINECS No.	202-088-8
TSCA Name	Benzenamine, N,N-diethyl-
Molecular Formula	C10H15N

Producer Related Part	
Company:	
Creation date:	15-JUL-1999

Substance Related Part	
Company:	
Creation date:	15-JUL-1999

Memo:	Bayer Corporation

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Number of Pages:	46

Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD and Company Information

Type: lead organisation
Name: American Chemistry Council (formerly Chemical Manufacturers Association), Monocyclic Aromatic Amines and Nitro Aromatics (MAANA) HPV Panel
Street: 1300 Wilson Boulevard
Town: 22209 Arlington, VA
Country: United States

17-AUG-2001

Type: cooperating company
Name: Albemarle Corporation
Country: United States

24-SEP-2001

Type: cooperating company
Name: Bayer Corporation
Country: United States

24-SEP-2001

Type: cooperating company
Name: Buffalo Color
Country: United States

24-SEP-2001

Type: cooperating company
Name: First Chemical Corporation
Country: United States

24-SEP-2001

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information

Substance type: organic
Physical status: liquid
Purity: >= 99.3 % w/w
21-OCT-1999

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

ANILINE, N,N-DIETHYL-
09-SEP-1999

BENZENAMINE, N,N-DIETHYL-
09-SEP-1999

DIETHYLANILINE
09-SEP-1999

DIETHYLPHENYLAMINE
09-SEP-1999

N,N-DIETHYLAMINOBENZENE
09-SEP-1999

N,N-DIETHYLAMINOBENZOL
09-SEP-1999

N,N-DIETHYLBENZENAMINE
09-SEP-1999

1.3 Impurities

CAS-No:
EINECS-No:
EINECS-Name: Basic nitrogen
Contents: ca. 9.3 % w/w
21-OCT-1999

1.4 Additives
-

1.5 Quantity
-

1.6.1 Labelling
-

1.6.2 Classification
-

1.7 Use Pattern

Type: type
Category: Use in closed system
20-JAN-2000

Type: industrial
Category: Chemical industry: used in synthesis
20-JAN-2000

Type: use
Category: Intermediates
20-JAN-2000

1.7.1 Technology Production/Use
-

1.8 Occupational Exposure Limit Values
-

1.9 Source of Exposure
-

1.10.1 Recommendations/Precautionary Measures
-

1.10.2 Emergency Measures
-

1.11 Packaging
-

1.12 Possib. of Rendering Subst. Harmless
-

1.13 Statements Concerning Waste
-

1.14.1 Water Pollution
-

1.14.2 Major Accident Hazards
-

1.14.3 Air Pollution
-

1.15 Additional Remarks
-

1.16 Last Literature Search
-

1.17 Reviews
-

1.18 Listings e.g. Chemical Inventories
-

2.1 Melting Point

Value:	-38.8 degree C			
Method:	other: Handbook value			
GLP:	no data			
Testsubstance:	other TS: N,N-diethylaniline; purity not noted			
Reliability:	(2) valid with restrictions Data from Handbook or collection of data			
Flag:	Critical study for SIDS endpoint			
17-AUG-2001		(1)	(2)	(3)

2.2 Boiling Point

Value:	216.3 degree C at 1013 hPa			
Method:	other: Handbook value			
GLP:	no data			
Testsubstance:	other TS: N,N-diethylaniline; purity not noted			
Reliability:	(2) valid with restrictions Data from Handbook or collection of data			
Flag:	Critical study for SIDS endpoint			
17-AUG-2001				(2)
Value:	215.5 degree C			
Decomposition:	no			
Method:	other: Handbook value			
GLP:	no data			
Testsubstance:	other TS: N,N-diethylaniline; purity not noted			
Reliability:	(2) valid with restrictions Data from Handbook or collection of data			
Flag:	Critical study for SIDS endpoint			
17-AUG-2001			(4)	(3)
Value:	217.1 degree C at 1013 hPa			
17-AUG-2001				(1)
Value:	92.4 degree C at 13.333 hPa			
Decomposition:	no			
Method:	other: no data			
GLP:	no data			
Testsubstance:	other TS: N,N-diethylaniline; purity not stated			
17-AUG-2001				(5)

2.3 Density

Type: relative density
Value: .9307 g/cm3 at 20 degree C
Method: other: Handbook value
GLP: no data
Testsubstance: other TS: N,N-diethylaniline; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
17-AUG-2001 (2) (3)

Type: density
Value: .94 g/cm3 at 20 degree C
Method: other: Handbook value
GLP: no data
Testsubstance: other TS: N,N-diethylaniline; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
16-APR-2001 (1)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: 0.136 mm at 25 degree C
Method: other (measured)
GLP: no data
Test substance: N,N-diethylaniline; purity not noted
Reliability: (2) valid with restrictions
Data from handbook or collection of data
Flag: Critical study for SIDS endpoint
24-SEP-2001 (67)

Value: .2 hPa at 20 degree C
Method: other (measured): Handbook value
GLP: no data
Test substance: N,N-diethylaniline; purity not noted
Reliability: (2) valid with restrictions
Data from handbook or collection of data
Flag: Critical study for SIDS endpoint
24-SEP-2001 (1) (3)

Value: .18 hPa at 25 degree C
Method: other (measured)
GLP: no
Test substance: N,N-diethylaniline; purity not noted
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
24-SEP-2001 (6)

Value: .4 hPa at 30 degree C
Method: other (measured): Handbook value

GLP:	no data
Test substance:	N,N-diethylaniline; purity not noted
Reliability:	(2) valid with restrictions Data from Handbook or collection of data
Flag:	Critical study for SIDS endpoint
24-SEP-2001	(1) (3)

Value:	1 hPa at 44.3 degree C
Method:	other (measured): Handbook value
GLP:	no data
Test substance:	N,N-diethylaniline; purity not noted
Reliability:	(2) valid with restrictions Data from Handbook or collection of data
Flag:	Critical study for SIDS endpoint
24-SEP-2001	(7)

Value:	1.4 hPa at 50 degree C
Method:	other (measured): Handbook value
GLP:	no data
Test substance:	N,N-diethylaniline; purity not noted
Flag:	Critical study for SIDS endpoint
17-AUG-2001	(1)

2.5 Partition Coefficient

log Pow:	3.17 at 25 degree C
Method:	OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year:	1979
GLP:	no
Test substance:	N,N-diethylaniline; purity not noted
Result:	n-octanol-water Partition coefficient = 1491.54 log Pow = 3.17
Reliability:	(1) valid without restriction Guideline study
Flag:	Critical study for SIDS endpoint
17-AUG-2001	(8)

log Pow:	3.153
Method:	other (calculated): KOWWIN Program (v1.65)
Year:	1999
GLP:	no
Test substance:	molecular structure
Reliability:	(2) valid with restrictions Accepted calculation method
Flag:	Critical study for SIDS endpoint
17-AUG-2001	(9)

log Pow:	3.2
Method:	other (calculated): A. Leo, CLOGP-3.63 (1991) Daylight, Chemical Information Systems, Inc. Irvine, CA USA
Year:	
GLP:	no
Testsubstance:	other TS: molecular structure

Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
17-AUG-2001 (10) (11) (3)

log Pow: 3.31 - 4
Method: other (measured): see references
Year:
GLP: no data
Testsubstance: other TS: N,N-diethylaniline; purity not stated
17-AUG-2001 (12) (13) (14) (3)

2.6.1 Water Solubility

Value: 130 mg/l at 20 degree C
Qualitative: moderately soluble (100-1000 mg/L)
Method: other
GLP: no data
Testsubstance: other TS: N,N-diethylaniline; purity not stated
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
17-AUG-2001 (10) (3)

Value: = 14400 mg/l at 12 degree C
Qualitative: very soluble (> 10000 mg/L)
Method: other: Handbook value
GLP: no data
Testsubstance: other TS: N,N-diethylaniline; purity not noted
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
17-AUG-2001 (15) (3)

2.6.2 Surface Tension
-

2.7 Flash Point

Value: 79 degree C
Type: closed cup
Method: other: DIN 51758
Year:
16-APR-2001 (10)

2.8 Auto Flammability
-

2.9 Flammability

Result:
Remark: Ignition temperature: approx. 500 degree C
16-APR-2001 (10)

2.10 Explosive Properties
-

2.11 Oxidizing Properties
-

2.12 Additional Remarks

Remark: The BUA-report No. 40 includes further information
16-APR-2001

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1560000 molecule/cm3
Rate constant: = .0000000001642617 cm3/(molecule * sec)
Degradation: 50 % after .8 hour(s)
Method: other (calculated): AOP v1.89
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
17-AUG-2001 (9)

3.1.2 Stability in Water

Type: abiotic
Method: other: (calculated): Hydrowin v1.67
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Result: Hydrowin v1.67 cannot estimate a hydrolysis rate constant for this structure.
Reliability: (2) valid with restrictions
24-SEP-2001 (9)

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 106-49-0; 121-69-7.

3.1.3 Stability in Soil
-

3.2 Monitoring Data (Environment)
-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: air water soil sediment
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: BCF v2.13 Level III Fugacity Model

Year: 1999

Result:

Media	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	0.2	1.56	1000	5.19e-012
Water	22.3	900	1000	2.27e-009
Soil	76.8	900	1000	4.26e-009
Sediment	0.718	3.6e+003	0	1.73e-009

Persistence Time: 528 hr
Reaction Time: 605 hr
Advection Time: 4.11e+003 hr
Percent Reacted: 87.2
Percent Advected: 12.8
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
17-AUG-2001 (9)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge
Concentration: 100 mg/l
Degradation: 0 % after 28 day
Result: under test conditions no biodegradation observed
Method: OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year: 1983 GLP: yes
Test substance: other TS: N,N-diethylaniline; purity = 99.5 %
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
17-AUG-2001 (16)

Type: aerobic
Inoculum: predominantly domestic sewage, adapted
Concentration: .8 mg/l related to Test substance
Degradation: > 90 % after 20 day
Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year: 1977 GLP: no
Test substance: other TS: N,N-diethylaniline; purity not noted
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
17-AUG-2001 (10)

Type: aerobic
Inoculum: activated sludge
Concentration: 100 mg/l related to Test substance
Degradation: after 14 day
Result: under test conditions no biodegradation observed
Method: OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year: 1981 GLP: no
Test substance: other TS: N,N-diethylaniline; purity not noted
Remark: Method: "Biodegradation test of chemical substance by microorganisms etc." stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "301C, Ready Biodegradability: Modified MITI Test I" stipulated in the OECD Guideline for Testing of Chemicals (May 12, 1981).
Sludge conc.: 30 mg/l
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
17-AUG-2001 (17)

3.6 BOD5, COD or BOD5/COD Ratio

C O D

COD: 2346 mg/g substance

16-APR-2001 (10)

Year: 1983 GLP: yes
Concentration: 4 mg/l related to Test substance

Remark: BOD5 < 0.1 g/g
COD 1.28 g/g
16-APR-2001 (16)

3.7 Bioaccumulation

Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 56 day
Concentration: .02 mg/l
BCF: 17 - 125
Elimination:
Method: OECD Guide-line 305 C
Year: 1981 GLP: no data
Test substance: other TS: N,N-diethylaniline; purity not stated
Remark: Method: "Bioaccumulation test of chemical substance in fish and shellfish" stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "305C, Bioaccumulation: Degree of Bioconcentration in Fish" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).
17-AUG-2001 (17)

Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 56 day
Concentration: .2 mg/l
BCF: 44 - 161
Elimination:
Method: OECD Guide-line 305 C
Year: 1981 GLP: no data
Test substance: other TS: N,N-diethylaniline; purity not stated
Remark: Method: "Bioaccumulation test of chemical substance in fish and shellfish" stipulated in the Order Prescribing the Items of the Test Relating to the New Chemical Substance (1974, Order of the Prime Minister, the Minister of Health and Welfare, the MITI No. 1). This guideline corresponds to "305C, Bioaccumulation: Degree of Bioconcentration in Fish" stipulated in the OECD Guidelines for Testing of Chemicals (May 12, 1981).
17-AUG-2001 (17)

Species:
Exposure period:
Concentration:
BCF: 70.58
Elimination:
Method: other: BCF Program (v2.13)
Year: GLP: no
Test substance: other TS: molecular structure
Result: Log Kow (estimated) : 3.15
Log Kow (experimental): 3.31

Log Kow used by BCF estimates: 3.31

Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70

Estimated Log BCF = 1.849 (BCF = 70.58)
Reliability: (2) valid with restrictions

Accepted calculation method
17-AUG-2001 (9)

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type:	flow through
Species:	Pimephales promelas (Fish, fresh water)
Exposure period:	96 hour(s)
Unit:	mg/l Analytical monitoring: yes
LC50:	16.4
Method:	EPA OPP 72-1
Year:	GLP: no data
Test substance:	other TS: N,N-diethylaniline purchased from Aldrich Chemical Co., Milwaukee, WI; purity = 99%
Method:	pH was adjusted to approximate that of Lake Superior water (pH 7.8) with NaOH or HCL. Compound analyses were done by GLC: all exposure chambers at 0,24,48,72, and 96 hr. Fathead minnows used in this experiment were 34 days old and were cultured at USEPA Environmental Research Laboratory, Duluth, MN and University of Wisconsin - Superior campus. 10 fish/concentration and control. Behavior and toxic signs were noted at 4,24,48,72 and 96 hours.
Test condition:	Temperature = 25.1 degree C (+/-0.57); Dissolved oxygen = 7.0 mg/l; pH =7.74; hardness = 39.5 mg/l CaCO3; Tank volume = 1 liter; Concentrations (measured)= 6.15, 13.1, 20.6, 27.9, 33.9 mg/l.
Reliability:	(1) valid without restriction Guideline study
Flag:	Critical study for SIDS endpoint

17-AUG-2001 (18)

Type:	static
Species:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period:	96 hour(s)
Unit:	mg/l Analytical monitoring: no
LC50:	38.5
Method:	other
Year:	1983 GLP: yes
Test substance:	other TS: N,N-diethylaniline; purity = 99.5 %
Test condition:	Temperature: 15 degree C, pH 6.8-8.0, Oxygen conc.: 6.0-10.6 mg/l
Reliability:	(2) valid with restrictions Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag:	Critical study for SIDS endpoint

17-AUG-2001 (16)

Type:
Species: Oryzias latipes (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 25
Method: other: according to Japan Industrial Standards
Year: 1971 GLP:
Test substance: other TS: N,N-diethylaniline; purity not noted
Result: LC50 (24 hours) = 40.0 mg/l
Reliability: (2) valid with restrictions
19-JUN-2001 (8)

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
LC0: 20
LC100: 50
Method: other: Determination of the Acute Effect of Substances on Fish. "Fish Test" research group in the "Detergents" advisory committee (10/15/73)
Year: 1973 GLP: no
Test substance: other TS: N,N-diethylaniline; purity not stated
17-AUG-2001 (10)

Type:
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: 7.63
Method:
Year: GLP: no
Test substance: other TS: molecular structure
Remark: QSAR calculation
24-SEP-2001 (19)

Type: other: calculation
Species: other: Fish
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: 9.181
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
24-APR-2001 (9)

Type:
Species: Oryzias latipes (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
LC50: 16.8
Method: other: Japanese Industrial Standard (JIS K 0102-1986-71) "Testing methods for industrial waste water"
Year: GLP: no data
Test substance: other TS: N,N-diethylaniline; purity not stated
17-AUG-2001 (17)

Type:
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mol/l Analytical monitoring: no data
LC50: 3.959
Method: other: no data
Year: GLP: no data
Test substance: other TS: N,N-diethylaniline; purity not stated
17-AUG-2001 (20)

Type:
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: 6.14
Method:
Year: GLP: no
Test substance: other TS: molecular structure
Remark: QSAR calculation
17-AUG-2001 (19)

Type: other: calculation
Species: other: Fish
Exposure period: 14 day
Unit: mg/l Analytical monitoring: no
LC50: 19.963
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
24-APR-2001 (9)

4.2 Acute Toxicity to Aquatic Invertebrates

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring: no
EC0: 35.4
EC50: 70.7
EC100: 141
Method: OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year: 1984 GLP: no
Test substance: other TS: N,N-diethylaniline; purity not noted
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
17-AUG-2001 (10) (21)

Type: static
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: yes
EC50: 1 - 1.6
Method: EPA OTS 797.1300
Year: 1992 GLP: yes
Test substance: other TS: N,N-diethylaniline; purity >99%; supplied by Merck
Result:

	Nominal	Measured
EC50 -24hr	18mg/l(2.8-116)	3.5mg/l (0.25-25)
EC50 -48hr	7.7 mg/l (6.5-9.1)	1.3mg/l (1.0-1.6)

Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
24-SEP-2001 (22)

Type: static
Species: other: Tetrahymena pyriformis
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no data
EC50: 35.1
Method: other: according to Schultz, T. et al. (1991)
Year: GLP: no data
Test substance: other TS: N,N-diethylaniline; purity >95%
Result: Log of the inverse of 48hr 50% Inhibitory Growth Concentration (IGC50) = 3.629 mol/l
28-SEP-2001 (23)

Type: other: calculation
Species: Daphnia sp. (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 10.651
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
19-JUN-2001 (9)

Type: other: calculation
Species: Mysidopsis bahia (Crustacea)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50 : 1.165
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
24-APR-2001 (9)

Type: other: calculation
Species: Daphnia sp. (Crustacea)
Exposure period: 16 day
Unit: mg/l Analytical monitoring: no
EC50: .903
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
19-JUN-2001 (9)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Scenedesmus subspicatus (Algae)
Endpoint: other: cell count
Exposure period: 72 hour(s)
Unit: mg/l Analytical monitoring: no
EC10: 2.8
EC50: 5.6
Method: other: Determination of the inhibitory effect of substances in water on the green algae Scenedesmus-Cell multiplication inhibition- L 9, 1987g
Year: 1987 GLP: no
Test substance: other TS: N,N-diethylaniline; purity not noted

Reliability: (2) valid with restrictions
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
17-AUG-2001 (10) (24)

Species: other algae: green algae
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring:
EC50: 7.114
ChV : 1.383
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
17-AUG-2001 (9)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: activated sludge
Exposure period: 3 hour(s)
Unit: mg/l Analytical monitoring:
EC50: > 100
Method: other: ETAD 103: A Screening Test for the Assessment of the Possible Inhibitory Effect of a Chemical Substance on Aerobic Waste Water Bacteria (26.07.1979)
Year: GLP: no data
Test substance: other TS: N,N-diethylaniline; purity = 99.5 %
17-AUG-2001 (16)

Type: aquatic
Species: Pseudomonas fluorescens (Bacteria)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring: no
EC0: 1000
Method: other: Determination of the harmful biological effects of toxic sewage on bacteria. DEV, L 8 (1968) modified.
Year: 1973 GLP: no
Test substance: other TS: N,N-diethylaniline; purity not stated
17-AUG-2001 (10)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species: other
Endpoint: other
Exposure period: 30 day
Unit: mg/l Analytical monitoring: no
ChV : 1.424
Method: other: ECOSAR v0.99e
Year: GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
17-AUG-2001 (9)

4.5.2 Chronic Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Endpoint:
Exposure period: 21 day
Unit: mg/l Analytical monitoring: no
Method: other: UBA-Draft proceedings (preliminary report) "Chronic toxicity to Daphnia magna" (Determination of the NOEC for reproduction rate, mortality, and time point of the first occurrence of progeny, 21 d)(02/01/1984)
Year: GLP: no
Test substance:
Remark: R 21: 82.1 % at 0.3 mg/l
16-APR-2001 (10)

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

Type: other: calculation
Species: Eisenia fetida (Worm (Annelida), soil dwelling)
Endpoint: other
Exposure period: 14 day
Unit: other: ppm
LC50: 406.143
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Remark: Chemical may not be soluble enough to measure this predicted

effect.
Reliability: (2) valid with restrictions
Accepted calculation method
17-AUG-2001 (9)

4.6.2 Toxicity to Terrestrial Plants
-

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species
-

4.7 Biological Effects Monitoring
-

4.8 Biotransformation and Kinetics
-

4.9 Additional Remarks

Remark: BUA Report No. 40 includes further ecotoxicological data.
16-APR-2001

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Strain: Wistar
Sex: male
Number of Animals: 10
Vehicle: other: undiluted
Value: ca. 606 mg/kg bw
Method: Directive 84/449/EEC, B.1 "Acute toxicity (oral)"
Year: 1978 GLP: no
Test substance: other TS: undiluted N,N-diethylaniline; purity not noted
Method: single oral application by gavage of undiluted TS, 0.1, 0.5, 0.7, 0.8 ml/kg, 14 d observation period
Remark: LD50 = 0.65 ml/kg bw
Result: signs of toxicity: cyanosis, palmospasms, disorders of balance, increased diuresis, impaired general condition

Doses ml/kg	toxicological result no.of rats with toxic signs	no of deaths	time of death
0.1	0	0	
0.5	10	1/10	d 2
0.6	10	2/10	d 4-6
0.7	10	6/10	d 2-4
0.8	10	10/10	d 2-5

Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
17-AUG-2001 (25)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 720 mg/kg bw
Method:
Year: GLP: no
Test substance: other TS: undiluted N,N-diethylaniline

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: 720 - 1159 mg/kg bw
Method: other: no data
Year: GLP: no data
Test substance: no data
10-AUG-2000 (27)

Type: LD50
Species: rat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: = 782 mg/kg bw
Method:
Year: GLP: no data
Test substance:
16-APR-2001 (28)

Type: LDLo
Species: rabbit
Strain:
Sex:
Number of Animals:
Vehicle:
Value: 486 - 1870 mg/kg bw
Method: other: no data
Year: GLP: no data
Test substance: no data
10-AUG-2000 (27)

5.1.2 Acute Inhalation Toxicity

Type: LC50
Species: rat
Strain:
Sex:
Number of

Animals:	
Vehicle:	
Exposure time:	4 hour(s)
Value:	= 1.92 mg/l
Method:	other: according to: OECD Acute Toxicity Screening Program, Protocol for Acute Inhalation Toxicity Studies (modified)
Year:	GLP: yes
Test substance:	other TS: N,N-diethylaniline; purity not noted

Remark:	LC50 value expressed as actual exposure concentration (analytically determined) Particle size ~ 3.5 - 5.0 microns; 75-89% <10 microns
Result:	signs of toxicity (among others): ataxia and tremors in animals exposed to an actual concentration of 1.97 mg/l or greater
Reliability:	(1) valid without restriction GLP guideline study
Flag:	Critical study for SIDS endpoint

17-AUG-2001 (29)

5.1.3 Acute Dermal Toxicity

Type:	LD50
Species:	rat
Strain:	no data
Sex:	no data
Number of Animals:	
Vehicle:	other: undiluted
Value:	> 5000 mg/kg bw
Method:	other: undiluted TS, observation time: 14 d, no further information
Year:	GLP: no
Test substance:	other TS: undiluted N,N-diethylaniline; purity not noted
Remark:	no signs of intoxication, no local irritancy
Flag:	Critical study for SIDS endpoint

17-AUG-2001 (30)

Type:	LD50
Species:	rabbit
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	468 - 935 mg/kg bw
Method:	other: no data
Year:	GLP: no data
Test substance:	no data
Remark:	Mortality 0/4 at 468 mg/kg; 4/4 at 935 mg/kg.

16-APR-2001 (31)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: mouse
Strain:
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: = 870 mg/kg bw
Method:
Year: GLP: no
Test substance: other TS: undiluted N,N-diethylaniline
16-APR-2001 (32)

Type: LD50
Species: mammal
Strain:
Sex:
Number of Animals:
Vehicle:
Route of admin.: other: unreported
Value: = 2570 mg/kg bw
Method:
Year: GLP: no data
Test substance:
16-APR-2001 (33)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: slightly irritating
EC classificat.:
Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year: 1981 GLP: no data

Test substance: other TS: undiluted N,N-diethylaniline
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
17-AUG-2001 (34)

Species: rat
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: not irritating
EC classificat.:
Method: other: according to: Draize, J.P. et al.: J. of Pharmacol. 82, 377 (1944)
Year: GLP: no
Test substance:
Reliability: (2) valid with restrictions
16-APR-2001 (35)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result: moderately irritating
EC classificat.:
Method: other: site of application: back or ear; exposure time: 1 min., 5 min., 15 min. (back) and 20 hours (back or ear); observation period: 8 days
Year: GLP: no
Test substance: other TS: undiluted N,N-diethylaniline
16-APR-2001 (30)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of
Animals:
PDII:
Result:
EC classificat.:
Method: other: exposure time: 24 hours, site of application: ear, dose: 500 ul/animal, semiocclusive, observation period: 7 days
Year: GLP: no

Test substance:
Remark: result: highly irritating, corrosive
16-APR-2001 (36)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: not irritating
EC classificat.:
Method: OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year: 1987 GLP: no data
Test substance: other TS: undiluted N,N-diethylaniline; purity not noted
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
17-AUG-2001 (37)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: not irritating
EC classificat.:
Method: other: dose: 50 mg/animal, observation period: 8 days
Year: GLP: no
Test substance: other TS: undiluted N,N-diethylaniline
16-APR-2001 (30)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result:
EC classificat.:
Method: other: dose: 0.1 ml/animal (according to: Draize, J.P. et al.: J. of Pharmacol. 82, 377 (1944))
Year: GLP: no
Test substance: other TS: undiluted N,N-diethylaniline
Remark: result: little irritative effects (maximal effects 1 hour

after application); effects completely reversible after 48-96 hours
16-APR-2001 (35)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: slightly irritating
EC classificat.:
Method: other: dose: 100 ul/animal, observation period: 7 days
Year: GLP: no
Test substance:
16-APR-2001 (36)

5.3 Sensitization

Type: other
Species: guinea pig
Number of Animals:
Vehicle:
Result: not sensitizing
Classification:
Method: other: induction exposure by dermal application of a 10 % solution of N,N-diethylaniline; challenge exposure by dermal application of 1 or 2 % solutions of the test substance
Year: GLP: no
Test substance: other TS: N,N-diethylaniline was dissolved in acetone
Flag: Critical study for SIDS endpoint
16-APR-2001 (35)

Type: other
Species: human
Number of Animals:
Vehicle:
Result:
Classification:
Method:
Year: GLP:
Test substance: other TS: N,N-diethylaniline; commercial grade
Remark: No cases of allergic sensitization have been reported as a result of exposures at Buffalo Color Corporation.
Flag: Critical study for SIDS endpoint
16-APR-2001 (38)

5.4 Repeated Dose Toxicity

Species:	rat Sex: male/female
Strain:	Wistar
Route of admin.:	gavage
Exposure period:	28 d
Frequency of treatment:	daily, 7 d/w
Post. obs. period:	no
Doses:	10, 50 or 250 mg/kg bw/d
Control Group:	yes, concurrent vehicle
LOAEL:	10 mg/kg bw
Method:	OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"
Year:	1981 GLP: no data
Test substance:	other TS: N,N-diethylaniline; purity: 99.73 %
Result:	all dose groups: mortality and growth of the animals not significantly altered; food intake and water intake comparable to control values; haematology: decreased red cell counts, decreased haemoglobin contents, decreased packed cell volume (PCV) values in males and females, increased MCV- and MCH-values in the females; black colouration of the spleen; absolute and relative spleen weights increased; histological evidence of the spleen: haemosiderosis, extramedullary haematopoiesis, splenic hyperaemia; histological evidence of the liver: haemosiderosis in the Kupffers cells 10 mg/kg bw/d: no clinical signs of toxicity 10 and 50 mg/kg bw/d: no indications of nephrotoxic effects 50 mg/kg bw/d: increased frequency of respiratory sounds in the males 50 and 250 mg/kg bw/d: haematology: increased MCV- and MCH-values in the males, decreased MCHC-values in males and females, hyperbilirubinaemia; polychromasia; swollen spleens; histological evidence of the liver: increase in the extramedullary haematopoiesis 250 mg/kg bw/d: increased frequency of respiratory sounds in the females; increased salivation in the females; black colouration of the kidneys in the females; histopathological findings in the kidneys of males and females: ferriferous pigment detectable in the epithelia of the pars contorta; clinical chemistry of the peripheral blood: increased albumin levels in the males, decreased potassium levels in males and females
Reliability:	(1) valid without restriction Guideline study
Flag:	Critical study for SIDS endpoint

Species: dog Sex: no data
Strain: no data
Route of admin.: s.c.
Exposure period: 3 d
Frequency of treatment: no data
Post. obs. period: no
Doses: 5 g/animal (total dose given to the animal in the course of the experimental period)
Control Group: no data specified
Method:
Year: GLP: no
Test substance: other TS: N,N-diethylaniline was dissolved in olive oil
Remark: one animal was used in the study
Result: signs of toxicity (no details) on the second experimental day, death of the animal on the third day; p-diethylaminophenol identifiable as urinary metabolite; neither N,N-diethylaniline nor N,N-diethylaniline-N-oxide detectable in the urine
16-APR-2001 (40)

Species: rabbit Sex: no data
Strain: no data
Route of admin.: s.c.
Exposure period: 5 d
Frequency of treatment: no data
Post. obs. period: no
Doses: 2.9 g/animal (total dose given to the animals during the experimental period)
Control Group: no data specified
Method:
Year: GLP: no
Test substance: other TS: N,N-diethylaniline was dissolved in olive oil
Remark: 2 animals were used in the study
Result: signs of toxicity (no details) on the fourth experimental day, death of the animals 2 days later; p-diethylaminophenol identifiable as urinary metabolite; neither N,N-diethylaniline nor N,N-diethylaniline-N-oxide detectable in the urine
16-APR-2001 (40)

Species: guinea pig Sex: no data
Strain: no data
Route of admin.: s.c.
Exposure period: 5 h
Frequency of treatment: 4 s.c. injections within 5 h
Post. obs. period: no
Doses: total dose: 3000 mg/kg bw
Control Group: no
Method:
Year: GLP: no
Test substance:
Remark: 1 animal was used
Result: signs of toxicity: tremor, convulsions, paralysis of the pelvic extremities, nystagmus, accelerated respiration; death of the animal 4 hours after the final application
16-APR-2001 (41)

Species: guinea pig Sex: no data
Strain: no data
Route of admin.: s.c.
Exposure period: 33 h
Frequency of treatment: 9 s.c. injections within 33 h
Post. obs. period: no
Doses: total dose: 11000 mg/kg bw
Control Group: no
Method:
Year: GLP: no
Test substance:
Remark: 1 animal was used
Result: signs of toxicity: tremor, convulsions, paralysis of the pelvic extremities, decelerated and laboured respiration, blood not black-coloured
16-APR-2001 (41)

Species: rabbit Sex: no data
Strain: no data
Route of admin.: s.c.
Exposure period: 41.5 h
Frequency of treatment: 3 s.c. injections within 41.5 h
Post. obs. period: no
Doses: total dose: 1400 mg/kg bw
Control Group: no
Method:
Year: GLP: no
Test substance:
Remark: 1 animal was used
Result: no signs of toxicity following the first and the second application (administration of 300 and 500 mg/kg bw, respectively, at an interval of 17.5 hours); signs of toxicity following the third injection after further 24 hours: brownish discoloration of the pupils and of the blood, no central nervous effects; death occurred 26 hours after the third application due to a subacute feverish nephritis
16-APR-2001 (41)

Species: mouse Sex:
Strain:
Route of admin.: other: injection
Exposure period: 4 days
Frequency of treatment: 12 injections/day
Post. obs. period: No Data
Doses: 450 mg/kg/day
Control Group: no data specified
Method:
Year: GLP: no data
Test substance: no data
Remark: 10 out of 10 tumor-bearing mice failed to survive more than four days at 450 mg/kg/day. All of 10 tumor-bearing mice survived 12 daily injections of 225 mg/kg. May cause kidney and/or liver damage.
10-AUG-2000 (42)

Species: mouse Sex: no data
Strain: no data
Route of admin.: i.p.
Exposure period: 3 d
Frequency of treatment: daily
Post. obs. period: no data
Doses: 0.5 mM/kg bw/d (= 75 mg/kg bw/d)
Control Group: yes
Method:
Year: GLP: no
Test substance:
Result: forty-eight hours after the final administration, no significant methaemoglobin or sulphhaemoglobin formation was observed (no further data)
16-APR-2001 (43)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium TA 97, TA 100, TA 1535, TA 1537, TA 1538, TA 2637
Concentration: 1-5000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: modified preincubation method of the Ames assay
Year: GLP: no data
Test substance: other TS: N,N-diethylaniline; purity not noted
Reliability: (2) valid with restrictions
Guideline study with acceptable restrictions
Flag: Critical study for SIDS endpoint
17-AUG-2001 (44)

Type: Unscheduled DNA synthesis
System of testing: primary cultured rat hepatocytes
Concentration: 1 uM - 1 mM (= 0.15 - 150 ug/ml)
Cytotoxic Conc.:
Metabolic activation:
Result: negative
Method: OECD Guide-line 482 "Genetic Toxicology: DNA Damage and

Repair/Unscheduled DNA Synthesis in Mammalian Cells in vitro"
Year: GLP: no data
Test substance: other TS: N,N-diethylaniline; purity not stated
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
17-AUG-2001 (45)

Type: Escherichia coli reverse mutation assay
System of testing: Escherichia coli WP2 uvrA, WP2 uvrA/pKM
Concentration: 1-5000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: modified preincubation method of the Ames assay
Year: GLP: no data
Test substance: other TS: N,N-diethylaniline; purity not noted
Flag: Critical study for SIDS endpoint
17-AUG-2001 (44)

Type: Ames test
System of testing: Salmonella typhimurium TA 97, TA 98, TA 100, TA 1535
Concentration: 1-333 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: preincubation assay
Year: GLP: no data
Test substance: other TS: N,N-diethylaniline; label purity: 99 %
17-AUG-2001 (46)

Type: Bacterial gene mutation assay
System of testing: bacterial test system (no further data)
Concentration:
Cytotoxic Conc.:
Metabolic activation: no data
Result: negative
Method:
Year: GLP: no data
Test substance:
17-AUG-2001 (47)

Type: Ames test
System of testing: Salmonella typhimurium (no further data)
Concentration: no data
Cytotoxic Conc.:
Metabolic activation: no data

Result: negative
Method:
Year: GLP: no data
Test substance:
17-AUG-2001 (48)

Type: Ames test
System of testing: Salmonella typhimurium TA 98
Concentration: 1-5000 ug/plate
Cytotoxic Conc.:
Metabolic activation: without
Result: negative
Method: other: modified preincubation method of the Ames assay
Year: GLP: no data
Test substance: other TS: N,N-diethylaniline; purity not noted
Remark: the test was performed in the presence of norharman
24-SEP-2001 (44)

Type: Ames test
System of testing: Salmonella typhimurium TA 98
Concentration: 1-5000 ug/plate
Cytotoxic Conc.:
Metabolic activation: with
Result: positive
Method: other: modified preincubation method of the Ames assay
Year: GLP: no data
Test substance: other TS: N,N-diethylaniline; purity not noted
Remark: the test was performed in the presence of norharman
24-SEP-2001 (44)

5.6 Genetic Toxicity 'in Vivo'

Type: Micronucleus assay
Species: mouse Sex: male/female
Strain: other: Bor: NMRI (SPF Han)
Route of admin.: i.p.
Exposure period: single administration
Doses: 600 mg/kg bw
Result: negative
Method: OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year: GLP: yes
Test substance: other TS: N,N-diethylaniline; purity: 99.73 %
Result: no indications of a clastogenic effect of N,N-diethyl-aniline were found; there was an altered ratio between polychromatic and normochromatic erythrocytes
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint

5.7 Carcinogenicity
-

5.8 Toxicity to Reproduction

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 106-49-0; 108-44-1; 121-69-7.

5.9 Developmental Toxicity/Teratogenicity

Species:	rat Sex: female
Strain:	other: CD (Sprague-Dawley derived)
Route of admin.:	gavage
Exposure period:	days 6-15 of gestation
Frequency of treatment:	daily
Duration of test:	sacrifice of the females on day 20 of gestation
Doses:	50, 250 or 500 mg/kg bw/d
Control Group:	yes, concurrent vehicle
NOAEL Maternalt.:	250 ml/kg bw
NOAEL Teratogen.:	250 ml/kg bw
Method:	EPA OTS 798.4900
Year:	GLP: no data
Test substance:	other TS: N,N-diethylaniline; purity: 98.4 - 98.5 %
Remark:	the low- and mid-dose groups contained 24 females each; the high-dose group contained a total of 29 females
Result:	all dose groups: maternal effects: mean food consumption statistically lower than control; excessive salivation; no adverse effect of treatment evident from uterine implantation data; evaluation of fetuses recovered from treated group females for external, visceral and skeletal malformations indicated no adverse effect of treatment (no teratogenic or embryotoxic effects) 50 and 250 mg/kg bw/d: no maternal mortality; mean fetal weight and fetal sex distribution unaffected 250 and 500 mg/kg bw/d: maternal effects: excessive lacrimation; staining of the skin/fur in the ano-genital area 500 mg/kg bw/d: maternal toxicity: two females died and three females were killed in a moribund condition (mortality rate = 17.2 %); fetotoxicity: mean fetal weight statistically lower than control, increase in the incidence of fetuses with unossified sternebral elements (suggestive of a retardation in ossification)
Reliability:	(1) valid without restriction Guideline study
Flag:	Critical study for SIDS endpoint

Species: rat Sex: female
Strain: other: CD (Sprague-Dawley derived)
Route of admin.: gavage
Exposure period: days 6-15 of gestation
Frequency of treatment: daily
Duration of test: sacrifice of all surviving females on day 20 of gestation
Doses: 100, 250, 500, 750, 1000, 1500 or 2000 mg/kg bw/d
Control Group: yes, concurrent vehicle
Method: EPA OTS 798.4900
Year: GLP: no data
Test substance: other TS: N,N-diethylaniline; 98.4 % active ingredient
Remark: five females/group were used
type: range-finding study
Result: all dose groups: no external malformations were seen in fetuses
100, 250 or 500 mg/kg bw/d: maternal data: no mortality; reduced body weight gain during the day 6-15 treatment period; decrease in food consumption during the day 6-10 interval of the treatment period
250 and 500 mg/kg bw/d: maternal effects: staining of the fur in the anogenital area
500 and 750 mg/kg bw/d: mean fetal body weight data lower than control
750 mg/kg bw/d: three females were killed in a moribund condition after one to three days of treatment; only one female survived to day 20 sacrifice
1000 mg/kg bw/d: all five females were sacrificed in a moribund condition on day 7 of gestation; maternal toxicity: ataxia, labored/shallow breathing, prostrate posture, cooler body temperature
1500 and 2000 mg/kg bw/d: the first two females in each group died or were killed in a moribund condition on day 7 of gestation following a single treatment day; due to this mortality, the dose groups were terminated
Reliability: (2) valid with restrictions
17-AUG-2001 (51)

5.10 Other Relevant Information

Type: Biochemical or cellular interactions
Remark: in vitro assay: N,N-diethylaniline revealed no inhibitory effect on mouse cytosolic aldehyde dehydrogenase activity; test system: L1210/CPA cells (= murine leukemia cell lines resistant to cyclophosphamide)
07-MAY-1993 (52)

Type: Metabolism
Remark: dogs received a single intravenous injection of 108 mg/kg bw of N,N-diethylaniline hydrochloride; 2 hours after the application the N,N-diethylaniline-N-oxide concentration attained a maximum of ca. 5.5 ug N-oxide/ml blood (no further data)
16-APR-1993 (53)

Type: Metabolism
Remark: in an in vitro assay, the metabolism of N,N-diethylaniline (concentration: 5 umol) by rabbit liver microsomal preparations was studied; after 20 min. incubation, 7.8 % of the initial substrate concentration was mono-N-demethylated (formation of N-ethylaniline), 4.2 % was N-oxidated (formation of N,N-diethylaniline-N-oxide) and 8.6 % of the initial concentration of N,N-diethylaniline was metabolized otherwise (unidentified metabolites)
19-APR-1993 (54)

Type: Metabolism
Remark: in vitro assays: the oxidative dealkylation of N,N-diethylaniline by synthetic iron(III) porphyrin systems (as a model of cytochrome P-450) was studied; N-ethylaniline was found to be formed by oxidation of N,N-diethylaniline
19-APR-1993 (55) (56)

Type: Metabolism
Remark: in vitro assay: microsomes from pork liver homogenates were incubated with N,N-diethylaniline (concentration: 5.0 umoles/ml = ca. 750 ug/ml): the N-oxide of N,N-diethylaniline was formed only when the reaction medium was supplemented with flavin adenine dinucleotide (FAD)
27-APR-1993 (57)

Type: other
Remark: the effectiveness of various antidotes in the treatment of oral intoxication with N,N-diethylaniline was investigated in male rats; N,N-diethylaniline and the antidotes were given orally by gavage, the administration of the antidote following immediately the treatment with N,N-diethylaniline: the administration of cows milk, caster oil or liquid paraffin did not affect significantly the mean survival time of the animals; the application of activated charcoal as a 10 % aqueous suspension induced a significant prolongation of the mean survival time
05-MAY-1993 (58) (59) (60) (61) (62) (63)

Type: other: acute inhalation risk
Remark: rats were exposed to an atmosphere saturated with vapours of N,N-diethylaniline at 20 degrees Centigrade for 8 h; no signs of toxicity were observable, no deaths occurred; no pathological findings were detectable in the animals killed after the 14 d-observation period (the test substance exhibited only little volatility)
21-APR-1993 (64)

Type: other: acute inhalation toxicity
Remark: rats (number of animals unspecified) were exposed to N,N-diethylaniline at a concentration of 0.8 mg/l for 6 hours (whole-body exposure; test concentration analytically determined); no signs of toxicity were observable during the exposure period; during the observation period (14 days) no deaths occurred and no significant changes of body weights

were detectable
16-APR-2001 (35)

Type: other: haemotoxicity
Remark: dogs were injected i.v. with 108 mg/kg bw of N,N-diethylaniline hydrochloride (single administration); ca. 3 hours after application, the methaemoglobin concentration attained a maximum of ca. 40 % of the total blood pigment; in an additional experiment, N,N-diethylaniline-N-oxide was found to display only minimal methaemoglobin-forming activity; thus the authors conclude that N,N-diethylaniline-N-oxide can be ruled out almost completely as the factor in the methaemoglobin formation following the injection of N,N-diethylaniline; the authors suppose that another metabolite of N,N-diethylaniline, namely p-diethylaminophenol, plays an important role in the methaemoglobin formation following the absorption of N,N-diethylaniline (this assumption has not yet been experimentally verified)
19-APR-1993 (53)

Type: other: haemotoxicity
Remark: after administration of lethal doses of N,N-diethylaniline to cats, methaemoglobin was detectable in blood samples (no further data)
16-APR-2001 (40)

Type: other: haemotoxicity
Remark: cats (1 male, 1 female) received a single oral administration of 50 ul/kg bw (= ca. 47 mg/kg bw) of N,N-diethylaniline; cyanosis was detectable and 4 h after application the maximal methaemoglobin level of blood was found to be 77.8 %; after 48 hours the methaemoglobin levels had returned to normal; the following further signs of toxicity were observed: abdominal position, apathy, vomiting, salivation (the effects had disappeared after 1 day); in this study, the methaemoglobinaemic activity of N,N-diethylaniline was comparable to that of aniline
26-APR-1993 (65)

Type: other: haemotoxicity
Remark: after a single i.p. administration of 0.5 mM/kg bw (= 75 mg/kg bw) of N,N-diethylaniline to mice, methaemoglobin formation was induced; a maximum concentration of ca. 15 % methaemoglobin was reached 10 min. after application; 24 hours after the administration the concentration of methaemoglobin was comparable to control values; a significant sulphhaemoglobin formation was not observable at any time

5. Toxicity

Type:
Remark: N,N-diethylaniline was administered to rats orally (doses: 180 - 2100 mg/kg bw) or i.p. (doses: 280 - 2100 mg/kg bw) or percutaneously (doses: 7100 - 16000 mg/kg bw) (single administrations; 1 animal/dose used); the lowest lethal dose was found to be 620 mg/kg bw given orally and 420 mg/kg bw given i.p.; even the highest dose given percutaneously (16000 mg/kg bw) did not induce deaths (the authors suppose that in the case of percutaneous application the relatively volatile test substance was not completely absorbed); the following signs of toxicity were observable in the experiments: cyanosis, clonic spasms, uraemia; at higher doses: unconsciousness, lateral position, small enlargement of the liver; histological findings (at higher doses): degeneration and necrosis of the renal tubular epithelium; granular degeneration of the liver cells
16-APR-2001 (35)

Type:
Remark: N,N-diethylaniline given orally to rats (single administration) revealed almost no methaemoglobinaemic activity, in comparison with aniline (no further data)
16-APR-2001 (66)

5.11 Experience with Human Exposure

Remark: Due to the considered adequacy of the engineering controls, routine atmospheric monitoring sufficient to result in statistically significant statements on exposure control has not been carried out. Raised methaemoglobin levels have not been observed in personnel operating the plant, thus the confidence in the controls in place has been confirmed by the lack of observed effects.
16-APR-2001

(1) Auer-Technikum, Auergesellschaft mbH Berlin, 12. Ausg. 1988

(2) CRC Handbook of Chemistry and Physics. 80th edition (1999-2000) David R. Lide, ed. CRC Press, New York. p 3-21 No. 695.

(3) Verschueren, K. (2001) Handbook of Environmental Data on Organic Chemicals, 4th Edition. volume 2. John Wiley & Sons: New York. pps 835-6.

(4) Perry and Chilton. (1973) Chemical Engineer's Handbook, 5th Edition. McGraw-Hill, New York.

(5) Verschueren, K. (1983)

(6) Walton, J. et al, Eng. Sci. Data Item 78011, 1-30 (1978)

(7) CRC Handbook of Chemistry and Physics. 80th edition (1999-2000) David R. Lide, ed. CRC Press, New York. p 6-88.

(8) Tonogai, Y. et al., The J. of Toxicological Sciences 7, 193-203 (1982)

(9) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510

(10) BUA Report No. 40, VCH, October 1989

(11) Calculation Bayer AG, WV-UWS/Produktsicherheit (1992)

(12) Sangster, J. 1989. J. Phys. Chem. Ref. Data 18(3):1111-1207

(13) Schultz OE, Jung C, Loeller KE. 1970. Z. Naturforscher B. 25:1024

(14) THOR database Pomona 91, Daylight, Chemical Information Systems, Inc. Irvine, CA, USA

(15) American Cyanamid Company; National Safety Council.

(16) Zeneca Brixham Environmental Laboratory, Study No. KO34A (1983)

(17) Biodegradation and Bioaccumulation Data of Existing

Chemicals Based on the CSCL Japan, Compiled under the Supervision of Chemical Products Safety Division, Basic Industries Bureau MITI, Ed. by CITI, October 1992. Published by Japan Chemical Industry Ecology-Toxicology & Information Center

(18) Geiger DL, Poirier SH, Brooke LT, Call DJ. (eds) 1986. Acute toxicities of organic chemicals to fathead minnows (pimephales promelas) Vol III. Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI. p. 245-6

(19) Hutzinger, O. et al., Utility of the QSAR Modeling System for Predicting the Toxicity of Substances on the European Inventory of Existing Commercial Chemicals, Preliminary Report to VCI, 1988

(20) Schultz, T. (1991)

(21) Neuhahn. Bayer AG. January 21, 1988.

(22) Pedersen F, Bjornestad E, Vulpius T, Rasmussen HB. 1998. Report to Danish EPA. Immobilisation Test of Aniline Compounds with the Crustacean Daphnia magna. VKI ATV Project No. 303587. GLP Study No. 308209/609-625.

(23) Schultz, T. et al. (1991) Science of Total Environ. 109/110: 581-587

(24) Neuhahn & Hamburger. Bayer AG. February 26, 1988

(25) Loeser, E. Bayer AG data, short report, May 26, 1978

(26) Hazleton Laboratories Europe: Acute oral LD50 in the rat. test article XXVI 486, Report for BASF AG (1978)

(27) Scientific Associates Report, SA 98084. (January 20, 1965)

(28) Marhold, J.: Prehled Prumyslove Toxikologie. Organicke Latky. Svazek 1 (Praha, 1986), p. 465

(29) Voss, K.A. et al.: Food and Drug Research Laboratories, unpublished report No. 6771 D, date: November 2, 1981, submitted to: Buffalo Color Corporation (West Paterson, NJ/USA)

(30) BASF AG, Abteilung Gewerbehygiene und Toxikologie: Bericht ueber die gewerbetoxikologische Grundpruefung (1979)

(31) Scientific Associates Report, SA. 98084 (January 20, 1965): Letter K.H. Ferber/J.E. Loughlin, February 1, 1965.

(32) Hazleton Laboratories Europe: Acute intraperitoneal LD50

in the mouse. test article XXVI 486, Report for BASF AG (1978)

(33) Krasovskii, G.N. et al.: Gig. Sanit. 48(6), 22-25 (1983)

(34) Schreiber, G.: data of the Fraunhofer-Institut fuer Toxikologie und Aerosolforschung: Bericht ueber die Pruefung von N,N-Diethylanilin auf primaere Hautreizwirkung, October 27, 1982 (at the request of Bayer AG)

(35) Sziza, M. and Podhragyai, L.: Archiv fuer Gewerbepathologie und Gewerbehygiene 15, 447-456 (1957)

(36) Thyssen, J.: Bayer AG data, short report, October 2, 1978

(37) Schreiber, G.: data of the Fraunhofer-Institut fuer Toxikologie und Aerosolforschung: Bericht ueber die Pruefung von N,N-Diethylanilin auf Schleimhautreizwirkung, October 27, 1982 (at the request of Bayer AG)

(38) Buffalo Color Corporation, Health Hazard Summary and Evaluation of Commercial Grade Chemicals: N,N-diethylaniline.

(39) Bayer AG data, Report No. 22486, 1993/Sept/06

(40) Horn, F.: Hoppe-Seylers Z. Physiol. Chem. 249, 82-84 (1937)

(41) Vittinghoff, W.: Inaugural-Dissertation zur Erlangung der Doktorwuerde, Pharmakologisches Institut der Universitaet zu Marburg (1894)

(42) Hazardline, 1986; Wisconsin Alumni Research Foundation, 1958.

(43) Nomura, A.: Nippon Yakurigaku Zasshi 73, 423-435 (1977)

(44) Shimizu, H. and Takemura, N.: Occup. Health Chem. Ind., Proc. Int. Congr. 11th, 497-506 (1984)

(45) Yoshimi, N. et al.: Mutation Res. 206, 183-191 (1988)

(46) Zeiger, E. et al.: Environ. Molec. Mutagen. 11, Suppl. 12, 1-158 (1988)

(47) Japan Chemical Industry Ecology Toxicology & Information Center (JETOC): Newsletter 4, 13-20 (1985)

(48) National Toxicology Program, Annual Plan for Fiscal Year 1984, NTP-84-023, February 1984

(49) Bayer AG data, Report No. 21503, July 3, 1992

(50) BioDynamics Inc.: Project No. 85-2961 (BD-85-125), unpublished Final Report, submitted to Monsanto Company, November 20, 1986

(51) BioDynamics Inc.: Project No. 85-2958 (BD-85-124), unpublished Final Report, submitted to Monsanto Company, March 12, 1986

(52) Russo, J.E. et al.: Biochemical Pharmacology 37, 1639-1642 (1988)

(53) Kiese, M. et al.: Naunyn-Schmiedebergs Arch. Pharmak. u. exp. Path. 254, 253-260 (1966)

(54) Gorrod, J.W. et al.: Xenobiotica 9, 17-25 (1979)

(55) Miyata, N. et al.: Chem. Pharm. Bull. 29, 1489-1492 (1981)

(56) Santa, T. et al.: Chem. Pharm. Bull. 32, 1252-1255 (1984)

(57) Pettit, F.H. et al.: Biochem. Biophys. Res. Commun. 16, 444-448 (1964)

(58) Laass, W. and Kupfer, B.: Pharmazie 34, 114-115 (1979)

(59) Laass, W. and Wagner, H.: Pharmazie 32, 728-729 (1977)

(60) Laass, W. et al.: Pharmazie 32, 542 (1977)

(61) Laass, W.: Pharmazie 28, 65-66 (1973)

(62) Laass, W.: Pharmazie 28, 684-685 (1973)

(63) Laass, W.: Pharmazie 29, 728-729 (1974)

(64) BASF AG, Abteilung Gewerbehygiene und Toxikologie: Bericht ueber die Pruefung der akuten Inhalationsgefahr (akutes Inhalationsrisiko) von Diethylanilin an Sprague-Dawley-Ratten (1979)

(65) BASF AG, Abteilung Gewerbehygiene und Toxikologie: Bericht ueber die Pruefung der methaemoglobinbildenden Wirkung von Diethylanilin und Anilin an der Katze (1977)

(66) Jodynis, J. et al.: Bromat. Chem. Toksykol. 10(2), 151-155 (1977)

(67) Danner, R.P., Physical and Thermodynamic Properties of Pure Chemicals, Design Inst. Phys. Prop. Data. Amer. Inst. Chem. Eng. NY; NY: Hemisphere Pub. Corp. Vol. 1 (1991); Daubert, T.E. and Danner, R.P., (1991), in EPISUITE v. 3.10, physical properties of N,N-diethylaniline.

7. Risk Assessment

7.1 End Point Summary

-

7.2 Hazard Summary

-

7.3 Risk Assessment

-

D a t a S e t

Existing Chemical	Substance ID: 62-53-3
CAS No.	62-53-3
EINECS Name	aniline
EINECS No.	200-539-3
TSCA Name	Benzeneamine
Molecular Weight	93.13
Molecular Formula	C6H7N

2. Physico-chemical Data

2.1 Melting Point

Value:	-6.2°C
Reference:	BASF AG, Sicherheitsdatenblatt Anilin (04.01.1994)

2.2 Boiling Point

Value:	184.0°C
Reliability:	(1) valid without restriction
Flag:	**robust summary**
Reference:	BASF AG, Sicherheitsdatenblatt Anilin (04.01.1994)

2.3 Density

Type:	relative density
Value:	1.0213 at 20°C
Reliability:	(1) valid without restriction
Flag:	**robust summary**
Reference:	BASF AG, Sicherheitsdatenblatt Anilin (04.01.1994)

2.4 Vapour Pressure

Value:	0.49 mm
Temperature:	25°C
Method:	calculated[ ]; measured [x]
GLP:	Yes[ ] No[ ] ?[ ]
Remarks:	
Reference:	Danner, R.P., Physical and Thermodynamic Properties of Pure Chemicals, Design Inst. Phys. Prop. Data. Amer. Inst. Chem. Eng. NY; NY: Hemisphere Pub. Corp. Vol. 4 (1989); Daubert, T.E. and Danner, R.P., (1985), in EPISUITE v. 3.10, physical properties of aniline.

2.5 Partition Coefficient

log Pow: 0.91
Method:
Year:

Reference: BASF AG, Sicherheitsdatenblatt Anilin (04.01.1994)

2.6.1 Water Solubility

Value: 36 g/l at 20°C
pH: 8.8 at 36 g/l and 20°C
Reference: BASF AG, Sicherheitsdatenblatt Anilin (04.01.1994)

3.1.1 Photodegradation
Type: Air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Rate constant: .00000000011 cm3/(molecule * sec)
Method Measured
Year: GLP: no
Test Substance:
Remark: Concentration of sensitizer: about 10e10 molecule/cm3
Tropospheric half-lifetime 3.5 h calculated from the measured degradation constant, assuming a tropospheric OH radical concentration of 5 x 10e5 radicals/ml
Test condition: Absolute rate technique, OH radicals are monitored as a function of time after the pulsed flash lamp by resonance fluorescense detection system (RF)
Reference: Witte, F. et al, J. Phys. Chem. 90, 3251-3259 (1986).

Type: Air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Rate constant: .000000000118 cm3/(molecule * sec)
Method Measured
Year: GLP: no
Test Substance:
Remark: Concentration of sensitizer: 10e11 – 10e13 molecule/cm3
Tropospheric half-lifetime 3.26 h calculated from the measured degradation constant, assuming a tropospheric OH radical concentration of 5 x 10e5 radicals/ml
Test condition: Absolute rate technique, OH radicals are monitored as a function of time after the pulsed flash lamp by resonance fluorescense detection system (RF)
Reference: Atkinson, R., Chem. Rev. 85, 69-201 (1985).

3.1.2 Stability in Water
Type: Abiotic (hydrolysis) [x]; biotic (sediment) [ ]
Degradation: 11.3±9.9% at pH approx. 6.0 at 30°C after 48 hours.
Method: Schultz, T.W. et al, Bull. Environ. Toxicol. Chem. 42, 192-198 (1989);Yoshioka, Y. et al, Sci. Total Environ. 43, 149-157 (1985).

GLP: Yes[ ] No[x] ?[ ]
Remarks: Concentration tested was 71 mg/L.
Reference: Arnold, L.M. et al, Chemosphere 21 (1-2), 183-191 (1990).

3.5 Biodegradation

Type: aerobic
Inoculum: BASF-activated sludge
Concentration: 596 mg/l related to DOC (Dissolved Organic Carbon)
Degradation: 97 % after 5 days
Method: Modified OECD Screening Test
Year: GLP: no
Test substance: no data
Reference: BASF AG, Ecology Laboratory, unpublished research: Biotic Degradation: Modified OECD Screening Test of 6/5/81.

Type: aerobic
Inoculum: BASF-activated sludge
Concentration: 100 mg/l related to DOC (Dissolved Organic Carbon)
Degradation: 92 % after 6 days
91% after 3 days
39% after 1 day
15% after 3 hours
Method: Standard experimental method
Year: 1980 GLP: no
Test substance: no data
Reference: BASF AG, Ecology Laboratory, unpublished research: Biotic Degradation: Standard experimental method of 5/6/80.

3.7 Bioaccumulation

Species: Brachydanio rerio (fish, fresh water); static
Exposure period: 24 hours
Concentration: 2 µg/l
BCF: 2.6 $\pm$ 0.27
GLP: No data
Remark: Uptake constant was 11.1 $\pm$ 3.2/h. Aniline concentrations were measured via HPLC.
Reference: Zok, S., Sci. Total Environ. 109/110, 411-421 (1991).

Species: Selenastrum capricornutum (Algae)
Exposure period: 24 hours
Concentration: 0.36 mg/l and 2 mg/l
BCF: 91
GLP: No data
Reference: Hardy, J.T. et al., Environ. Toxicol. Chem. 4, 29-35 (1985).

4.0 Ecotoxicity

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)

Unit: mg/l Analytical monitoring:
EC50: .25
Method: Flow-through
Year: GLP: no data
Test substance:
Test condition: 17.2 degrees Centigrade; pH 7.4
Reference: Holcombe, G.W. et al., Arch. Environ. Contam. Toxicol. 16, 697-710 (1987).

Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
EC0: .01
EC50: .3
EC100: 1.2
Method: Daphnia Short Term Test, DIN 38412 Part 11, Determination of the Effect of Substances in Water on Crustacea
Year: GLP: no
Test substance:
Reference: Kuehn, R. et al., Research report: Harmful effects of environmental chemicals in the Daphnia Reproduction Test as a basis for the verification of environmental hazards in aquatic systems (UFOPLAN Nr. 1063052). Berlin (1988).

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Chlorella pyrenoidosa (Algae)
Endpoint: growth rate
Exposure period: 72 hours
Unit: mg/l Analytical monitoring: yes
EC50: 94-175
Method: OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year: 1984 GLP: no data
Test substance: purity: 99.5% (Merck, Darmstadt, Germany)
Reference: Ramos, E.U. et al, Aquatic Toxicology 46, 1-10 (1999).

Species: Selenastrum capricornutum (Algae)
Endpoint: growth rate
Exposure period: 96 hours
Unit: mg/l Analytical monitoring:
EC50: 19
Method: EPA algal growth inhibition test
Year: 1971 GLP: no
Test substance:
Reference: Calamari, D. et al., Chemisphere 9, 753-762 (1980).

5. Toxicity

5.4 Repeated Dose Toxicity

Species: rat Sex: male
Strain: Fischer 344

Route of admin.: oral gavage; no vehicle
Exposure period: 5, 10, or 20 Days
Frequency of treatment: daily
Post. obs. period: none
Dose: 110 mg/kg body weight per day
Control Group: yes; sham dosed
Method: Described in the publication
Year: GLP: no data
Test substance: 99.9% purity (MCB Chemicals)
Result: Deaths, decreased body weights(5 days) and increased spleen weights; transient cyanosis after dosing; rough hair coat; splenic congestion, increased hematopoiesis and hemosiderosis, and bone marrow hyperplasia.
Comments: Blood changes were consistent with enhanced erythrocyte destruction.
Reference: Short, C.R. et al, Fundam. Appl. Toxicol. 3, 285-292 (1983).

Species: rat Sex: male
Strain: no data
Route of admin.: inhalation
Exposure period: 2 weeks
Frequency of treatment: 3, 6, or 12 hr/day, 5 days/week
Post. obs. period: 14 days
Doses: 0, 10, 30, or 90 ppm
Control Group: yes
NOAEL: 10 ppm
Test substance:
Result: At $\geq$ 30 ppm: concentration dependent effects, splenic congestion, hemolysis, increased MCV, MCHb and methemoglobin values; methemoglobin values were normal within 14 days after exposure, and spleen values were nearly normal.
Comments: Concentration, not time, was the primary determinant to use in setting exposure limits
Reference: Burgess, B.A. et al., The Toxicologist 4, p. 64 [A] (1984).

5.5 Genetic Toxicity 'in Vitro'

Type: Cytogenetic assay
System of testing: Chinese hamster lung (CHL) fibroblast cells
Concentration: 1000 ug/ml
Metabolic activation: with and without
Result: positive with activation at 1000 ug/ml and higher
Method: Ishidate Jr., M. (Ed.) (1987) Chromosomal Aberration Test in Vitro, L.I.C., Inc., Tokyo.
Year: GLP: no data
Test substance:

Reference: Ishidate,Jr., M., et al., (1988): Mutat. Res. 195, 151-213.

Type: Cytogenetic assay
System of testing: Chinese hamster (v79) cells
Concentration:
Metabolic activation: with and without
Result: positive
Method:
Year: GLP: no data
Test substance:
Reference: Miltenburger, H.G., Test report of study LMP 102. Laboratory for mutagenicity testing, Technical University Darmstadt (1986); on behalf of BG Chemie, Heidelberg.

Type: Cytogenetic assay
System of testing: Chinese hamster ovary (CHO) cells
Concentration: 160 to 1600 ug/ml without activation; 500 to 5000 ug/ml with activation
Metabolic activation: with and without
Result: weak positive with activation at 5000 ug/ml only
Method: Galloway et al (1985)
Year: GLP: no data
Test substance: obtained from NTP chemical repository
Reference: Galloway, S.M. et al, Environ. Mol. Mutagen. 10 (Suppl. 10), 1-175 (1987).

Type: Cell transformation
System of testing: Balb/3T3
Concentration: 0.8, 4, 20, and 100 ug/ml
Metabolic activation: none
Result: positive
Method: Kakunaga, T., Int. J. Cancer 12, 463-473 (1973).
Year: GLP: no data
Test substance: supplied by the NCI Chemical Repository
Reference: Dunkel, V.C. et al, J. Nat. Cancer Inst. 67(6), 1303-1315 (1981).

Type: Cell transformation
System of testing: SHE
Concentration: 0.05, 0.50, and 5.0 ug/ml
Metabolic activation: none
Result: negative
Method: Freeman, A.E. et al, J. Nat. Cancer Inst.51, 799-808 (1973); Pienta, R.J. et al, in: Nieburgs HE, et al, eds., Cancer Prevention and Detection. Part 1. Vol 2

New York: Marcel Dekker, 1978:1993-2011; DiPaolo, J.A. et al, Cancer Res. 31, 1118-1127 (1971).

Year: GLP: no data

Test substance: supplied by the NCI Chemical Repository

Reference: Dunkel, V.C. et al, J. Nat. Cancer Inst. 67(6), 1303-1315 (1981).

5.6 Genetic Toxicity 'in Vivo'

Type: Cytogenetic assay
Species: mouse Sex: male and female
Strain: SJL Swiss
Route of admin.: intraperitoneal
Exposure period: single administration; animals killed after 24 hr
Doses: 0, 5, 50, 100, and 200 mg/kg bw
Method: no data; method described in publication
Year: GLP: no data
Test substance: Purified by recrystallization or distillation
Result: positive
Reference: Sicardi, S.M., et al., J. Pharm. Sci. 80(8), 761-764 (1991).

Type: Cytogenetic assay
Species: mouse Sex: male
Strain: CRH
Route of admin.: oral
Exposure period: single administration; animals killed after 24 and 48 hr
Doses: 0, 400, 500, and 1000 mg/kg bw
Method: given in publication
Year: GLP: no data
Test substance: hydrochloride salt, purity >99%
Result: positive at 1000 mg/kg
Reference: Westmoreland, C. and Gatehouse, D.G., Carcinogenesis 12(6), 1057-1059 (1991).

Type: Cytogenetic assay
Species: rat Sex: male
Strain: PVG
Route of admin.: oral gavage
Exposure period: single administration;animals killed after 24 and 48 hr
Doses: 0, 215, 287, 400, and 500 mg/kg body weight
Method: Schmid, W., Mutat. Res. 31, 9-15 (1975).
Year: GLP: no data
Test substance: hydrochloride salt
Result: Positive
Reference: George, E. et al.,Carcinogenesis 11(9), 1551-1555 (1990).

Type: Cytogenetic assay
Species: mouse Sex: male
Strain: CBA
Route of admin.: intraperitoneal
Exposure period: two injections 24 hr apart; animals killed after 24 and 48 hr

Doses:	experiment 1: 0,100, 200, 250, and 300 mg/kg body weight Experiment 2: 0, 237.5, and 380 mg/kg body weight
Method:	Schmid, W., Mutat. Res. 31, 9-15 (1975).
Year:	GLP: no data
Test substance:	AnalaR grade material used; redistilled
Result:	Positive
Reference:	Ashby, J., et al., Mutat. Res. 263, 115-117 (1991).

Type:	Dominant lethal assay
Species:	rat
Strain:	Alpk:ApfSD (Wistar-derived)
Route of admin.:	intraperitoneal
Exposure period:	5 consecutive days
Doses:	0, 75, 150, 200 mg/kg body weight
Result:	No evidence of a dominant lethal effect
Method:	OECD Guideline 478 “Genetic Toxicology: Rodent Dominant Lethal Test”
Year:	1998 GLPL yes
Test substance:	purity 99.9%
Remark:	methyl methane sulphonate (MMS) used as positive control was clearly positive
Reference:	Milburn, G.M. Central Toxicology Laboratory report no. CTL/P/5404: Aniline: Dominant Lethal Study in the Rat, 4/17/98 (at the request of the Aniline Association Inc.)

5.7 Carcinogenicity

Species:	rat Sex: male and female
Strain:	F344
Route of admin.:	oral feed
Exposure period:	104 weeks
Frequency of Treatment:	daily
Post. Obs. Period:	none
Doses:	0, 10, 30, or 100 mg/kg body weight
Control Group:	yes
Method:	
Year:	GLP:
Test substance:	hydrochloride salt
Result:	Decreased mean hematocrit, hemoglobin, and erythrocytes in mid- and high-dose males and high-dose females. Increased absolute/relative spleen weights in mid- and high-dose males and females. Stromal hyperplasia and fibrosis of the splenic red pulp in high-dose melas and, to a lesser degree, in females. Chronic capsulitis in high-dose animals. Increased incidence of primary splenic sarcomas principally in high dose males (males: 0, 0, 1.3, and 37.8%; females: 0, 0, 0, and 1.3%).
Reference:	Anon., 104-Week chronic toxicity study in rats, aniline hydrochloride. CIIT, Research Triangle Park, USA (1982); Bus, J.S., and Popp, J.A., Fd. Chem. Toxicol. 25(8), 619-626 (1987).

Species: rat Sex: male and female
Strain: F344
Route of admin.: oral feed
Exposure period: 103 weeks
Frequency of Treatment: daily
Post. Obs. Period: low dose 4 weeks; high dose 5 weeks; control 7 weeks
Doses: 0, 3000, or 6000 ppm in diet
Control Group: yes
Method:
Year: GLP:
Test substance: hydrochloride salt
Result: 17/25, 34/50 and 27/50 males and 16/25, 44/50 and 41/50 females survived on test until the end of the study. Slight mean body weight depression in treated females and high-dose males. Increased incidence of splenic or abdominal fibrosarcomas and sarcomas. The incidence of combined sarcomas and fibrosarcomas was 0/25, 5/50 and 18/48 in males and 0/24, 1/50 and 7/50 in females. Splenic hemangiosarcomas were significantly increased in males (0/25, 19/50 and 21/48).
Reference: Anon., Bioassay of aniline hydrochloride for possible carcinogenicity, CAS No. 142-04-1, technical report series no. 130 (NTIS PB-287539). Nat. Cancer Inst., Bethesda, 67 p. (1978).

Species: mouse Sex: male and female
Strain: B6C3F1
Route of admin.: oral feed
Exposure period: 103 weeks
Frequency of Treatment: daily
Post. Obs. Period: low and high dose 4 weeks; control 6 weeks
Doses: 0, 6000, or 12000 ppm in diet
Control Group: yes
Method:
Year: GLP:
Test substance: hydrochloride salt
Result: 33/50, 43/50, and 41/50 males and 30/50, 37/50, and 41/49 females survived on test until the end of the study. Mean body weight depression in dosed males. No increased incidence of tumors was observed in males or females when compared with control animals.
Reference: Anon., Bioassay of aniline hydrochloride for possible carcinogenicity, CAS No. 142-04-1, technical report series no. 130 (NTIS PB-287539). Nat. Cancer Inst., Bethesda, 67 p. (1978).

5.9 Developmental Toxicity/Teratogenicity

Species: rat Sex: female
Strain: F344
Route of admin.: oral gavage
Exposure period: days 7-20 of gestation

Frequency of treatment: once per day
Doses: 0, 10, 30, or 100 mg/kg body weight
Control Group: yes
Method: given in publication
Year: GLP: yes
Test substance: hydrochloride salt; Eastman Kodak Co.
Remark: minimum of 20 rats/dose group.
Result: dams: ≥10 mg/kg: dose-dependent increase in relative spleen weights
dams: 100 mg/kg: significant increases in methemoglobin and hematopoietic activity
fetuses: 100 mg/kg: increased relative liver weights and hematopoietic activity
Reference: Price, C.J. et al, Toxicol. Appl. Pharmacol. 465-478 (1985).

Species: rat Sex: female
Strain: F344
Route of admin.: oral gavage
Exposure period: gestation day 7 through parturition
Post-exposure obs. period: Pup development was followed from birth to postnatal day 60
Frequency of treatment: once per day
Doses: 0, 10, 30, or 100 mg/kg body weight
Control Group: yes
Method: given in publication
Year: GLP: yes
Test substance: hydrochloride salt; Eastman Kodak Co.
Remark: 15-16 litters/treatment group.
Result: dams (killed on postnatal day 30): 100 mg/kg: significant increase in relative spleen weights, methemoglobin, and red blood cell size
fetuses: ≥10 mg/kg: dose-related increase in postnatal deaths
fetuses: ≤ 30 mg/kg: increased relative liver weights
fetuses: 100 mg/kg: significant increase in red blood cell size; reduced body weights
Reference: Price, C.J. et al, Toxicol. Appl. Pharmacol. 465-478 (1985).

I U C L I D

D a t a S e t

Existing Chemical	ID: 121-69-7
CAS No.	121-69-7
EINECS Name	N,N-dimethylaniline
EINECS No.	204-493-5
TSCA Name	Benzenamine, N,N-dimethyl-
Molecular Formula	C8H11N

2. Physico-chemical Data ID: 121-69-7

2.1 Melting Point

Value:	2.4 degree C
Reference:	CRC Handbook of Chemistry and Physics, 80th ed, p 3-24 (1999).

2.2 Boiling Point

Value:	= 194.1 degree C
Reference:	CRC Handbook of Chemistry and Physics, 80th ed, p 3-24 (1999).

2.3 Density

Type:	density
Value:	= .9557 g/cm3 at 20 degree C
Reference:	CRC Handbook of Chemistry and Physics, 80th ed, p 3-24 (1999).

2.4 Vapour Pressure

Value:	= 0.70 mm at 25 degree C
Reference:	Danner, R.P., Physical and Thermodynamic Properties of Pure Chemicals, Design Inst. Phys. Prop. Data. Amer. Inst. Chem. Eng. NY; NY: Hemisphere Pub. Corp. Vol. 4 (1989).

2.5 Partition Coefficient

log Pow:	= 2.28
Method:	other (calculated): Inkrementenmethode von Rekker mit Computerprogramm der Firma CompuDrug Ltd.
Year:	
Reference:	BASF AG, Labor fuer Umweltanalytik; unveroeffentlichte

Untersuchung (09.01.1989)

2. Physico-chemical Data ID: 121-69-7

2.6.1 Water Solubility

Value: = 1.2 g/l at 20 degree C
pH: 7.4 at 1.2 g/l and 20 degree C
Reference: BASF AG, Sicherheitsdatenblatt N,N-Dimethylanilin (06.01.1994)

3. Environmental Fate and Pathways ID: 121-69-7

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
  Sensitizer: O3
  Degradation: = 50 % after 1.2 day
Method:
  Year: GLP:
Test substance: Purity 99%
Remark: Concentration of Sensitizer: $7.2X10^{-11}$ molecules/cm^3
Rate Constant: $9.1X10^{-18}$ cm^3/moleculeXsec
Test condition: Reaction vessel; temperature 296 K; reaction products: Hydrogen peroxide, formic acid, formaldehyde, N-methylformanilide
Reference: Atkinson,R. et al., Environ. Sci. & Technol.21, 64-72, (1987)

Type: air
INDIRECT PHOTOLYSIS
  Sensitizer: OH
  Conc. of sens.: 500000 molecule/cm^3
  Degradation: = 50 % after 2.6 hours
Method:
  Year: GLP:
Test substance: Purity 99%
Remark: Rate Constant: $1.48X10^{-10}$ cm^3/moleculeXsec
Test condition: Flash photolysis; fluorescent resonance; temperature range 278-464 K
Reference: Atkinson,R. et al., Environ. Sci. & Technol.21, 64-72, (1987)

Type: air
INDIRECT PHOTOLYSIS
  Sensitizer: OH
  Conc. of sens.: 3000000 molecule/cm3
Method:
  Year: GLP:
Test substance:
Remark: Atmospheric transformation: lifetime less than 1 day
Reference: Kelly,T.J. et al., Environ. Sci. Technol.28, 378-387, (1994)
Type: air

INDIRECT PHOTOLYSIS
  Sensitizer: HNO3 (Gasphase)
  Degradation: = 50 % after 1.6 day

Method:
  Year: GLP:
Test substance: Purity 99%
Remark: Concentration of Sensitizer: 2.6 ug/m^3
Rate Constant: $\geq 2X10^{-16}$ cm^3/moleculeXsec
Test condition: Reaction vessel
Reference: Atkinson,R. et al., Environ. Sci. & Technol.21. 64-72, (1987.)

Type: air
INDIRECT PHOTOLYSIS
  Sensitizer: HNO3 (Gasphase)
  Degradation: = 50 % after 1.6 day
Method:
  Year: GLP:
Test substance: Purity 99%
Remark: Concentration of Sensitizer: 2.6 ug/m^3
Rate Constant: $\geq 2X10^{-16}$ cm^3/moleculeXsec
Test condition: Reaction vessel
Reference: Atkinson,R. et al., Environ. Sci. & Technol.21. 64-72, (1987.)

Type: water
INDIRECT PHOTOLYSIS
  Sensitizer: OH
  Degradation: = 50 % after 15 day
Method:
  Year: GLP:
Test substance:
Remark: Concentration of Sensitizer: 10^{-16} mol/l
Rate Constant: $5.3X10^9$ cm^3/moleculeXsec
Test condition: 25° C; pH 9
Reference: Anbar,M. et al., J. Phys. Chem.70, 2660-2662, (1966)

3.5 Biodegradation

Type: aerobic
Inoculum: bacteria: BASF activated sludge, adapted
Concentration: 95.5 mg/l related to test substance
Degradation: = 75 % after 28 day
Method: Directive 84/449/EEC, C.7 "Biotic degradation - modified MITI test"
  Year: GLP:
Test substance:
Remark: Degree of biodegradation based on the BSB/THSB ratio
Biological degradation processes are possible.
Potentially biologically degradable
Reference: BASF AG, Ecology Laboratory; unpublished research, (1991)

Type: aerobic
Inoculum: bacteria: activated sludge, not adapted/municipal
Degradation: < 10 % after 28 day
Method: Directive 84/449/EEC, C.7 "Biotic degradation - modified MITI test"
  Year: GLP:
Test substance:
Remark: Initial concentration: 50/100/200 mg/l (test substance)
BSB of CSB
Reference: BASF AG, Ecology Laboratory; unpublished research, (1985)

Type: aerobic
Inoculum: activated sludge

Degradation: ca. 65 % after 28 day
Result: readily biodegradable
Method: OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year: 1983 GLP: yes
Test substance:
Reference: Zeneca, Hedset for EUCLID

Type: aerobic
Inoculum: activated sludge
Concentration: 100 mg/l related to Test substance
Degradation: = 95 % after 28 day
Method: OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year: 1983 GLP: yes
Test substance:
Remark: 95% bioelimination (DOC removal)
Reference: Zeneca, Hedset for EUCLID

Type: aerobic
Inoculum: bacteria: activated sludge, adapted/industrial
Concentration: 400 mg/l
Degradation: = 100 % after 6 days
Method: OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year: GLP:
Test substance:
Remark: Initial concentration based on TOC
Results point to evaporation and adsorption as elimination mechanisms.
Evidence of biological degradation processes are not given.
The concentration lies in the range of inhibition of the respiratory activity of activated sludge.
Reference: BASF AG, Ecology Laboratory; unpublished research, (1986)

Type: aerobic
Inoculum: bacteria: adapted inoculum
Degradation: = 22 % after 5 day
Method: BSB-Test (BSB to THSB)
Year: GLP:
Test substance:
Remark: In addition BSB5 to THSB = 0%; no information on inoculum.
Reference: Niemi,G.J. et al., Environ. Toxicol. Chem.6, 515-527, (1987)

3.7 Bioaccumulation

Species: Carassius auratus (Fish, fresh water)
Exposure period: 48 hours
Concentration: 808 mg/l
BCF: = 6.8
Elimination:
Method:
Year: GLP:
Test substance:
Remark: The tested concentrations of 80/90/100/200/300 mg/l
Were ranged over the LC50 value of Fischart.
The DMA content in fish did not go up proportionally with the concentration in water, but remained constant, once the animals were torpid. Not until after death did the concentration in the fish change.
Reference: Ogawa,S. et al., Eisei Kagaku 29, 286-291, (1983)

Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 42 day at 25 degree C
Concentration: .05 mg/l
BCF: ca. 4.7 - 10.1
Elimination:
Method: OECD Guide-line 305 C "Bioaccumulation: Test for the Degree of Bioconcentration in Fish"
Year: GLP:
Test substance:
Reference: Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan, edited by Chemicals Inspection & Testing Institute Japan, published by Japan Chemical Industry Ecology-Toxicology & Information Center, October 1992

Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 42 day at 25 degree C
Concentration: .5 mg/l
BCF: ca. 5.4 - 13.6
Elimination:
Method: OECD Guide-line 305 C "Bioaccumulation: Test for the Degree of Bioconcentration in Fish"
Year: GLP:
Test substance:
Reference: Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan, edited by Chemicals Inspection & Testing Institute Japan, published by Japan Chemical Industry Ecology-Toxicology & Information Center, October 1992

Species: Cyprinus carpio (Fish, fresh water)
Exposure period: 48 hour(s)
Concentration: 80 mg/l
BCF: = 8.7
Elimination:
Method:
Year: GLP:
Test substance:
Remark: The tested concentrations of 80/90/100/200/300 mg/l were ranged over the LC50 value of Fischart.
The DMA content in fish did not go up proportionally with the concentration in water, but remained constant once the animals were torpid. Not until after death did the concentration in the fish change.
Reference: Ogawa, S. et al., Eisei Kagaku 29, 286-291, (1983)

4.2 Acute Toxicity to Aquatic Invertebrates

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring:
EC0: = .8
EC50: = 5
EC100: = 20
Method: Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year: GLP:
Test substance:
Test condition: Tested with 100 mg/l Tween 80 as a solvent.
Reference: BASF AG, Ecology Laboratory; unpublished research, (1020/88)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species:	Agmenellum quadruplicatum (Algae)
Endpoint:	
Exposure period:	
Unit:	Analytical monitoring:
Method:	Growth inhibition test
Year:	GLP:
Test substance:	
Remark:	No toxicity at 1000 ug/disk.
Reference:	Batterton,J. et al., Science 199, 1068-1070, (1978)

Species:	Scenedesmus subspicatus (Algae)
Endpoint:	
Exposure period:	96 hour(s)
Unit:	mg/l Analytical monitoring:
EC10:	= 210
EC50:	= 340
Method:	Scenedesmus cell multiplication inhibition, DIN 38412 Level 9, Determination of the inhibitory effect of water soluble substances on green algae.
Year:	GLP:
Test substance:	
Test condition:	Tested with 100 mg/l Tween 80 as solvent
Reference:	BASF AG, Ecology Laboratory; unpublished research, (1020/88)

5.4 Repeated Dose Toxicity

Species:	rat Sex: male/female
Strain:	Fischer 344
Route of admin.:	gavage
Exposure period:	14 days
Frequency of treatment:	daily
Post. obs. period:	no data
Doses:	93.75, 187.5, 375, 750 or 1500 mg/kg/day in corn oil.
Control Group:	yes, concurrent vehicle
NOAEL:	< 93.75 mg/kg
Method:	NTP study comparable to guideline study.
Year:	GLP: yes
Test substance:	N,N-dimethylaniline of purity >98%.
Remark:	Five males and 5 females were used in each group. All animals survived doses of 93.75 to 375 mg/kg; all animals, apart from one male, died 6 days after a dose of 750 mg/kg and all animals died at the highest dose after 3 days. Symptoms observed were: cyanosis, lethargy, slight tremor, diarrhea, discharge from nose and eyes. Splenomegaly was observed in 2 males and 1 female dosed with 93.75 mg/kg, in all animals apart from 1 female in the 187.5 mg/kg dose group, and in all animals in group given 375 mg/kg. One surviving male rat in the group given 750 mg/kg also showed splenomegaly. Extramedullary haematopoiesis and hemosiderosis were observed in the spleen of 3 males and 3 females given the dose of 375 mg/kg.
Reference:	NTP, Technical Report No. 360, NIH Publ. No 90-2815, PB 90-227240, 1989.

Species:	rat Sex: male/female
Strain:	Fischer 344

Route of admin.: gavage
Exposure period: 13 weeks
Frequency of treatment: 5 days/week
Post. obs. period: no data
Doses: 31.25, 62.5, 125, 250 or 500 mg/kg dissolved in 5 ml corn oil/kg
Control Group: yes, concurrent vehicle
NOAEL: < 31.25 mg/kg
Method: NTP study, comparable to guideline study.
Year: GLP: yes
Test substance: N,N-dimethylaniline of purity >98%.
Remark: Ten males and 10 females were used in each group. No compound-related mortality was noted. A significant decrease in body weight gain was observed in male rats at 250 and 500 mg/kg. Cyanosis was seen in rats of these two groups. Animals with splenomegaly were found in all dose groups. Bone marrow hyperplasia and increased hematopoiesis in the spleen occured. The severity of these lesions was dose-related.
Reference: NTP, Technical Report No. 360, NIH Publ. No 90-2815, PB 90-227240, 1989.

Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 15 days
Frequency of treatment: daily
Post. obs. period: no data
Doses: 93.75, 187.5, 375, 750 and 1500 mg/kg/day in corn oil.
Control Group: yes, concurrent vehicle
NOAEL: = 93.75 mg/kg bw
LOAEL: = 187.5 mg/kg bw
Method: NTP study, comparable to OECD guideline 407.
Year: GLP: yes
Test substance: N,N-dimethylaniline of purity >98%.
Remark: Five males and 5 females were used in each group, except that the dose of 187.5 mg/kg/day was given to 4 males. The doses of 93.75, 187.5 and 375 mg/kg were survived by all animals. In groups given higher doses (750 and 1500 mg/kg), all animals died after 12 days and 3 days, respectively. Symptoms observed were: lethargy, marked salivation and tremor. Splenomegaly was observed in 1 male dosed with 187.5 mg/kg and in 2 males and 3 females given the dose of 375 mg/kg. Haematoma and extramedullary haematopoiesis or haemosiderosis were observed in 3 males and 3 females in the group given 375 mg/kg.
Reference: NTP, Technical Report No. 360, NIH Publ. No 90-2815, PB 90-227240, 1989.

Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 13 weeks
Frequency of treatment: 5 days/week
Post. obs. period: no data
Doses: 31.25, 62.5, 125, 250 or 500 mg/kg in 10 ml corn oil/kg;

Control Group: yes, concurrent vehicle
NOAEL: = 31.25 mg/kg
LOAEL: = 62.5 mg/kg
Method: NTP study, comparable to guideline study.
Year: GLP: yes
Test substance: N,N-dimethylaniline of purity >98%.
Remark: Ten males and 10 females were used in each group. No substance-related mortality was demonstrated. The final mean body weight of male and female mice were within 12% of those of vehicle controls. Compound-related clinical signs included lethargy and salivation. Splenomegaly was observed in all dose groups; the severity was dose related, although reported to be minimal in 4/10 mice at the 31.25 mg/kg/day dose level. Extramedullary hematopoiesis and hemosiderosis occured in the spleen of dosed mice. The severity of these lesions was dose-related, although reported to be mild in 1/10 mice at the 31.25 mg/kg/day dose level.
Reference: NTP, Technical Report No. 360, NIH Publ. No 90-2815, PB 90-227240, 1989.

5.5 Genetic Toxicity 'in Vitro'

Type: Chromosomal aberrations
System of testing: Chinese hamster ovary cells
Concentration: up to 1010 ug/ml
Cytotoxic Conc.:
Metabolic activation: with and without
Result: Without S9 mix: positive in the highest dose only.
Source: BASF AG Ludwigshafen
Method: other: no data
Year: GLP: yes
Test substance: N,N-dimethylaniline of purity >98%.
Remark: NTP study.
Reference: Loveday K.S. et al. Envir. Mol. Mutagen. 13:60-94, 1989; Rosenkranz H. S. et al. Environ. Mol. Mutagen. 16:149-177, 1990; NTP, Technical Report No. 360, NIH Publ. No 90-2815, PB 90-227240, 1989;

Type: Micronuclei induction
System of testing: Chinese hamster V79 cells
Concentration: up to 0.14 mg/ml
Cytotoxic Conc.:
Metabolic activation: without
Result: Aneugenic effect: weak positive (2.5 times higher than in the negative control).
Method: Bonatti S. et al. Mutagen. 7:111-114
Micronuclei formation was matched with an immunofluorescent staining for kinetochore protein (CREST-antibodies).
Year: 1992 GLP: no data
Test substance: Purity of 99%.
Reference: Taningher M. et al. Environ. Mol. Mutagen. 21:349-356, 1993

5.7 Carcinogenicity

Species: rat Sex: male/female
Strain: Fischer 344
Route of admin.: gavage

Exposure period: 2 years
Frequency of treatment: 5 days/week for 103 weeks
Post. obs. period: no data
Doses: 3 or 30 mg/kg/day in corn oil
Control Group: yes, concurrent vehicle
Method:
Year: GLP: no data
Test substance: N,N-dimethylaniline of purity >98%.
Result: Groups of 50 rats of each sex were used. Mean body weights of vehicle control and dosed rats were comparable throughout the studies. The survival of rats among all respective groups was similar, except for the lower survival of vehicle control female rats (vehicle control, 21/50; low dose, 32/50; high dose, 36/50). Final survival for male rats were: 29/50; 32/50; 28/50, respectively.
Fatty metamorphosis and fibrosis in the spleen of high dose male rats were increased: 0/49; 1/49; 10/50, and 5/49; 2/49 and 22/50, respectively. SPLENIC HEMOSIDEROSIS and HEMATOPOIESIS were present at an incidence greater than 85% in all groups; however, the severity of lesions was greater in dosed groups than in controls. SACROMAS OF THE SPLEEN were seen in 3/50 high dose male rats, and an OSTEOSARCOMA was seen in another high dose male rat. One additional high dose male rat had a sarcoma of the thymus. Splenic sarcomas are uncommon in corn oil vehicle control male Fisher 344/N rats (0.1%); thus, these neoplasms were considered to be chemically related.
LOWER INCIDENCES OF MONONUCLEAR CELL LEUKEMIA (which apparently originates in the spleen) were seen in experimental male and female rats than in vehicle controls (male: 13/50; 4/50; 3/50, respectively; female: 11/50; 7/50; 0/50, respectively).
NTP study.
Reference: NTP, Technical Report No. 360, NIH Publ. No 90-2815, PB 90-227240, 1989.

Species: mouse Sex: male/female
Strain: B6C3F1
Route of admin.: gavage
Exposure period: 2 years
Frequency of treatment: 5 days/week for 103 weeks
Post. obs. period: no data
Doses: 15 and 30 mg/kg/day in corn oil
Control Group: yes, concurrent vehicle
Method: NTP
Year: GLP: no data
Test substance: N,N-dimethylaniline of purity >98%.
Result: Groups of 50 mice of each sex were used. Mean body weights of vehicle control and experimental mice were similar throughout the study. Final survival was as follows: male mice - vehicle control: 34/50; low dose: 30/50; high dose: 34/50; female mice - 35/50; 39/50; 33/50.
The incidence of squamous cell papillomas of the forestomach in high dose female mice was marginally greater than in vehicle controls (2/50; 2/50; 8/50).
No other effects were seen.
NTP study.
Reference: NTP, Technical Report No. 360, NIH Publ. No 90-2815, PB

90-227240, 1989.

5.9 Developmental Toxicity/Teratogenicity

Species:	mouse Sex: female
Strain:	CD-1
Route of admin.:	gavage
Exposure period:	8 days
Frequency of treatment:	8 consecutive days, Day 7 through Day 14 of gestation (vaginal plug = day 0)
Duration of test:	up to postnatal day 3
Doses:	365 mg/kg/day
Control Group:	yes, concurrent vehicle
Method:	Chernoff N. and Kavlock R.J. In: Short-term bioassays in the analysis of complex environmental mixtures, Ed. Waters et al. New York, Plenum Publishing Co. Vol. III: 417-427
Year:	1983 GLP: yes
Test substance:	N,N-dimethylaniline; no further data.
Results:	Fifty female mice were used. Three females died during the first 4 days after exposure; this effect was considered compound-related. No significant effect on maternal body weight or litter weight 3 days postpartum was observed. Three dams died; there were no deaths in the control group. Seven dams in the NN-dimethylaniline group and nine in the control group were not pregnant. Three dams in the treated group, but none in the control group, had been fertilized without subsequent implantation. One dam in the treated group had a dead litter which was not delivered by day 23 of gestation. Treatment with NN-dimethylaniline had no apparent effect on time to delivery and on reproduction outcome which was 97%. The average number of live pups per litter at birth was 9 ± 3 for the control group and 9 ± 3 for the treated group. The average number of live pups per litter 3 days postpartum was 8 ± 3 for the treated group and 9 ± 3 for the control group. Although the Offspring Viability Ratio was reported to be significantly (Student's t-test) reduced in the treated group compared with the control group, the reported mean ratios for treated (0.98 ± 0.04) and control (1.00 ± 0.02) group do not appear to be different.
Reference:	Hardin B.D. et al. Teratogen. Carcinogen. Mutagen. 7:29-48, 1987.

D a t a S e t

Existing Chemical	Substance ID: 108-44-1
CAS No.	108-44-1
EINECS Name	m-toluidine
EINECS No.	203-583-1
Molecular Weight	107.2
Molecular Formula	C7H9N

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2. Physico-chemical Data

2.1 Melting Point

Value: -31.2°C
Reference: CRC Handbook of Chemistry and Physics, 80th ed, p 3-24 (1999).

2.2 Boiling Point

Value: 203.3°C
Reference: CRC Handbook of Chemistry and Physics, 80th ed, p 3-24 (1999).

2.3 Density

Type: relative density
Value: .9889 at 20°C
Reference: CRC Handbook of Chemistry and Physics, 80th ed, p 3-24 (1999).

2.4 Vapour Pressure

Value: 0.303 mm
Temperature: 25°C
Method: calculated[ ]; measured [x]

GLP: Yes[ ] No[ ] ?[ ]
Reference: Chao, J. et al., J. Phys. Chem. Ref. Data 19(6), 1547-1615 (1990).

2.5 Partition Coefficient
log Pow: 1.40
Method: calculated[ ]; measured [x]
Year:
GLP: Yes[ ] No[ ] ?[X]
Reference: Fujita, T. et al, J. Amer. Chem. Soc 86, 5175 (1964).

2.6.1 Water Solubility
Value: 12 g/l at 20°C
pH:

Reference: Angelescu, C., Buletinul de chimie pura si aplicata Vol. 3, 32-49 (1941/42).

3.1.2 Stability in Water

Type: Abiotic (hydrolysis) [x]; biotic (sediment) [ ]
Degradation: 8.0±2.4% at pH approx. 6.4 at 30°C after 48 hours.
Method: Schultz, T.W. et al, Bull. Environ. Toxicol. Chem. 42, 192-198 (1989);Yoshioka, Y. et al, Sci. Total Environ. 43, 149-157 (1985).
GLP: Yes[ ] No[x] ?[ ]
Remarks: Concentration tested was 285 mg/L.
Reference: Arnold, L.M. et al, Chemosphere 21 (1-2), 183-191 (1990).

3.5 Biodegradation

Type: aerobic
Inoculum: mainly secondary effluent
Concentration: 20 mg/l related to DOC (Dissolved Organic Carbon)
Degradation: 64-84% after 28 days
Method: Modified OECD Screening Test, OECD Guide-line 301 E adopted May 12 84, Directive 84/449/EEC, C.3; ISO 7824 (1984).
Year: GLP:
Test substance:
Remark: degradation measured as DOC decrease, 2 parallels (64% and 84% degradation, respectively); recovery = 57% DOC in a separate test
Reference: Trenel, J., and Kuehn, R. Bewertung wassergefaehrdender Stoffe im Hinblick auf Lagerung, Umschlag und Transport und Untersuchung zur Abklaerung substanz- und bewertungsmethodenspezifischer Grenzfaelle bei der Bewertung wassergefaehrdender Stoffe, UFOPLAN des Bundesministers des Innern im Auftrag des Umweltbundesamtes, Juli 1982.

Type: aerobic
Inoculum: activated sludge, adapted
Concentration: 200 mg/l related to COD (Chemical Oxygen Demand)
Degradation: 97.7% after 5 days
Method: Batch system; inoculum concentratjion: 100 mg dry weight/l, 20 days adaptation
Year: GLP: no
Test substance: no data
Remark: degradation was measured as COD decrease
Reference: Pitter, P., Water Res. 10, 231-235 (1976).

4.0 Ecotoxicity

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Daphnia magna (Crustacea)
Exposure period: 48 hours
Unit: mg/l Analytical monitoring:
LC50: .75

Method: Concept NEN reports 6501 and 6502 from the Dutch Standard Organization (1980), mortality; static test
Year: GLP: yes
Test substance:
Remark: LC50 after correction of nominal concentrations for the average measured recoveries: 0.73 mg/l
Reference: Hermens, J. et al., Aquat. Toxicol. 5, 315-322 (1984).

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Scenedesmus quadricauda (Green algae)
Endpoint: growth rate
Exposure period: 96 hr
Unit: mg/l Analytical monitoring: no
Effect concentration 10
Method: German standard methods for the examination of water, wastewater, and sludge; bioassay (group L); determination of the inhibitory effects of water constituents on green algae (Scenedesmus cell multiplication inhibition test)(L9)
Year: GLP: no data
Test substance: no information
Reference: Bringmann, G, and Kuhn, R., Gesund. Ing. 80, 115-120 (1959); in AQUIRE.

Species: Scenedesmus subspicatus (Algae)
Endpoint:
Exposure period: 7 days
Unit: mg/l Analytical monitoring: no
Effect concentration: 6.1
Method: German standard methods for the examination of water, wastewater, and sludge; bioassay (group L); determination of the inhibitory effects of water constituents on green algae (Scenedesmus cell multiplication inhibition test)(L9)
Year: GLP: no
Test substance: no information
Remark: 57% recovery (DOC) in a separate test, initial pH = 7.5
Reference: Trenel, J. and Kuehn, R., Bewertung wassergefaehrdender Stoffe im Hinblick auf Lagerung, Umschlag und Transport und Untersuchung zur Abklaerung substanz- und bewertungsmethodenspezifischer Grenzfaelle bei der Bewertung wassergefaehrdender Stoffe, UFOPLAN des Bundesministers des Innern im Auftrag des Umweltbundesamtes, Juli 1982.

5. Toxicity

5.4 Repeated Dose Toxicity

Species: rat Sex: no data
Strain: no data

Route of admin.: gavage
Exposure period: 30 days
Frequency of treatment: daily
Post. obs. period: no data
Doses: 280 mg/kg/day
Control Group: yes
Method:
Year: GLP:
Test substance: no data
Result: decreased body weight, increased relative spleen weight, anemia (reduced oxygenated hemoglobin content, erythrocytopenia) increased sulfonated hemoglobin content, appearance of Heinz-Ehrlich bodies, decreased SH-groups in the blood, disturbed vitamin C content (no further data available).
Reference: Vasilenko, N.M. et al., Deposited Doc. ISS Viniti, 4035-4077 (1977).

5.7 Carcinogenicity

Species: rat Sex: male
Strain: Charles River CD
Route of admin.: oral feed
Exposure period: 78 weeks
Frequency of treatment: daily
Post. obs. period: 26 weeks
Doses: 8000 and 16000 ppm in diet for 13 weeks, then 4000 and 8000 ppm for 65 weeks
Control Group: yes; basal diet
Method: Described in publication
Year: GLP: no data
Test substance: Hydrochloride salt; purity checked by TLC and IR
Remark: Dosages were calculated to be 400 and 800 mg/kg body weight per day for the first 13 weeks and 200 and 400 mg/kg body weight per day for the last 65 weeks. 25 rats per group; histological examination was done on lungs, liver, spleen, kidney, adrenal, heart, bladder, stomach, intestine, reproductive organs, and pituitary.
Result: 400 and 800 mg/kg/day for 13 weeks let to a reduced body weight gain (10% and more) or death. Therefore, after 13 weeks the dosages were reduced to 200 and 400 mg/kg body weight per day for the remaining 65 weeks. No increase in tumors in treated animals.
Reference: Weisburger, E.K. et al, J. Environ. Pathol. Toxicol. 2, 325-356 (1978).

Species: mouse Sex: male and female
Strain: HaM/ICR
Route of admin.: oral feed
Exposure period: 18 months
Frequency of treatment: daily

Post. obs. period:	
Doses:	16000 and 32000 ppm in diet for 22 weeks (2400 and 4800 mg/kg of body weight); then 4000 and 8000 ppm for 56 weeks for males (600 and 1200 mg/kg of body weight), and 8000 and 16000 ppm for 56 weeks for females (1200 and 2400 mg/kg body weight)
Control Group:	yes; basal diet
Method:	Described in publication
Year:	GLP: no
Test substance:	Hydrochloride salt; purity checked by TLC and IR
Remark:	25 male and female mice per group; histological examination was done on lungs, liver, spleen, kidney, adrenal, heart, bladder, stomach, intestine and reproductive organs.
Result:	2400 and 4800 mg/kg body weight per day for 22 weeks led to a reduced body weight gain (10% and more) or death; after 22 weeks the doses were reduced for the remaining 56 weeks. Liver tumors were found in male mice, 4/16 examined at 600 mg/kg body weight per day; simultaneous controls had 1/18, and pooled control had 7/99.
Reference:	Weisburger, E.K. et al, J. Environ. Pathol. Toxicol. 2, 325-356 (1978).

D a t a S e t

Existing Chemical	Substance ID: 106-49-0
CAS No.	106-49-0
EINECS Name	p-toluidine
EINECS No.	203-403-1
Molecular Weight	107.2
Molecular Formula	C7H9N

---

2. Physico-chemical Data

2.1 Melting Point

Value: 43.7°C
Reference: CRC Handbook of Chemistry and Physics, 80th ed, p 3-24 (1999).

2.2 Boiling Point

Value: 200.4°C
Reference: CRC Handbook of Chemistry and Physics, 80th ed, p 3-24 (1999).

2.3 Density

Type: relative density
Value: .9619 at 20°C
Reference: CRC Handbook of Chemistry and Physics, 80th ed, p 3-24 (1999).

2.4 Vapour Pressure

Value: 0.286 mm
Temperature: 25°C
Method: calculated[ ]; measured [x]

GLP: Yes[ ] No[ ] ?[ ]
Reference: Chao, J. et al., J. Phys. Chem. Ref. Data 19(6), 1547-1615 (1990).

2.5 Partition Coefficient

log Pow: 1.39
Method: calculated[ ]; measured [x]
Year:
GLP: Yes[ ] No[ ] ?[X]
Reference: Fujita, T. et al, J. Amer. Chem. Soc 86, 5175 (1964).

2.6.1 Water Solubility

Value: 11 g/l at 20°C
pH: 7
Reference: Hoechst AG (1993): Safety Data Sheet p-Toluidine (24.02.1993)

3.1.2 Stability in Water
Type: Abiotic (hydrolysis) [x]; biotic (sediment) [ ]
Degradation: 8.8±0.2% at pH approx. 6.4 at 30°C after 48 hours.
Method: Schultz, T.W. et al, Bull. Environ. Toxicol. Chem. 42, 192-198 (1989);Yoshioka, Y. et al, Sci. Total Environ. 43, 149-157 (1985).
GLP: Yes[ ] No[x] ?[ ]
Remarks: Concentration tested was 113 mg/L.
Reference: Arnold, L.M. et al, Chemosphere 21 (1-2), 183-191 (1990).

3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge, industrial
Degradation: 94% after 8 days
Method: OECD Guide-line 302 B "Inherent biodegradabiltiy: Modified Zahn-Wellens Test"
Year: 1986 GLP: no
Test substance: no data
Reference: Wellens, H.Z., Wasser Abwasser Forsch. 23(3), 85-98 (1990).

Type: aerobic
Inoculum: activated sludge, adapted
Concentration: 200 mg/l related to DOC (Dissolved Organic Carbon)
Degradation: 97.7% after 5 days
Method: Batch system
Year: GLP: no
Test substance: no data
Remark: Inoculum 100 mg/l dry matter
Reference: Pitter, P., Water Res. 10, 231-235 (1976).

4.0 Ecotoxicity

4.2 Acute Toxicity to Aquatic Invertebrates

Species: Mysidopsis bahia (Crustacea)
Exposure period: 96 hours
Unit: mg/l Analytical monitoring: yes
EC50: 1.5
Method: USEPA TSCA Guideline 797.1930
Year: GLP: yes
Test substance: purity 99.5 %
Reference: First Chemical Corp. Study No. 13573.0695.6102.510

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: Scenedesmus quadricauda (Green algae)
Endpoint: growth rate
Exposure period: 96 hr
Unit: mg/l Analytical monitoring: no

EC0: <8
Method: static; see authors of this publication
Year: GLP: no data
Test substance: no information
Reference: Bringmann, G, and Kuhn, R., Gesund. Ing. 80, 115-120 (1959); in AQUIRE.

Species: Selenastrum capricornutum (Green algae)
Endpoint: growth rate
Exposure period: 14 days
Unit: mg/l Analytical monitoring: no
EC50: 0.203
Method: static
Year: GLP: no
Test substance: no information
Reference: Gaur, J.P., Acta Hydrochim. Hydrobiol. 16(6), 617-620 (1988); AQUIRE.

Species: Agmenellum quadruplicatum (Blue-green algae)
Endpoint: growth rate
Exposure period: 48 hr
Unit: Analytical monitoring: no
Method:
Year: GLP: no
Test substance: source was ChemService Inc. or MC&B Manufacturing Chemists
Remark: Strain PR 6 used. The addition of 50 ppb during exponential growth in a liquid culture resulted in a bending of the growth curve to a plateau within 4 hours. Cultures containing 500 ppb did not grow.
Reference: Batterton, J. et al., Science 199, 1068-1070 (1978).

5. Toxicity

5.4 Repeated Dose Toxicity

Species: rat Sex: male
Strain: no information
Route of admin.: oral feed
Exposure period: 4 weeks
Frequency of treatment: daily
Post. obs. period: none
Doses: 0, 165, 825, 1650 ppm (13.8, 66.8, 125.7 mg/kg body weight per day)
Control Group: yes
Method: T26-16:
Year: GLP: no
Test substance: no data
Remark: 10 animals/group
Result: At 1650 ppm of diet, there was decreased body weight gain. At 825 and 1650 ppm, there was also increased relative liver weight.
Reference: Industrial Bio-Test Laboratories Inc., BIO-FAX 31-4/73 (1973); cited in Documentation of TLVs and BEIs, ACGIH, 5th Ed. (1986).

5.5 Genetic Toxicity 'in Vitro'

Type:	Cytogenetic assay
System of testing:	Chinese hamster lung (CHL) fibroblast cells
Concentration:	500-1000 ug/ml
Metabolic activation:	with and without
Result:	positive with activation at 500 ug/ml and higher concentrations
Method:	
Year:	GLP: no data
Test substance:	no information
References:	Ishidate, Jr., et al., Mutat. Res. 195, 151-213 (1988)

5.6 Genetic Toxicity 'in Vivo'

Type:	Cytogenetic assay
Species:	mouse Sex: male and female
Strain:	Crl:CD-1®(ICR)BR
Route of admin.:	intraperitoneal
Exposure period:	One treatment
Doses:	43.75, 87.50, and 175.0 mg/kg body weight
Method:	OECD 474. Mammalian Erythrocyte Micronucleus Test
Year:	1997 GLP: yes
Remarks:	Cells were harvested at 24, 48, and 72 hr (fmales only at 72 hr, no males remaining). Signs of clinical toxicity and mortality were observed. 1000 immature erythrocytes were scored per animal instead of 2000. Individual body weights of animals are not given in the report, only ranges.
Test substance:	Purity was 99.8%
Result:	negative
Reference:	First Chemical Corp. Study No. 18136-0-455

5.7 Carcinogenicity

Species:	rat Sex: male
Strain:	Charles River CD
Route of admin.:	oral feed
Exposure period:	18 months
Frequency of treatment:	daily
Post. obs. period:	
Doses:	0, 1000, 2000 ppm in diet
Control Group:	yes; basal diet
Method:	Described in publication
Year:	GLP: no data
Test substance:	Hydrochloride salt; purity checked by TLC and IR
Remark:	25 rats per group
Result:	No increase in tumors in treated animals
Reference:	Weisburger, E.K. et al, J. Environ. Pathol. Toxicol. 2, 325-356 (1978).

Species:	mouse Sex: male and female
Strain:	HaM/ICR
Route of admin.:	oral feed
Exposure period:	18 months
Frequency of treatment:	daily
Post. obs. period:	
Doses:	0, 1000, 2000 ppm in diet for 6 months; then 500 and 1000 ppm for 12 months
Control Group:	yes; basal diet
Method:	Described in publication
Year:	GLP: no data
Test substance:	Hydrochloride salt; purity checked by TLC and IR
Remark:	25 mice per group
Result:	Increase in liver tumors in males at both dose levels and in females at the high dose level.
Reference:	Weisburger, E.K. et al, J. Environ. Pathol. Toxicol. 2, 325-356 (1978).

I U C L I D

D a t a S e t

Existing Chemical	ID: 103-69-5
CAS No.	103-69-5
EINECS Name	N-ethylaniline
EINECS No.	203-135-5
TSCA Name	Benzenamine, N-ethyl-
Molecular Formula	C8H11N

Producer Related Part	
Company:	
Creation date:	15-JUL-1999

Substance Related Part	
Company:	
Creation date:	15-JUL-1999

Memo:	Bayer Corporation

Printing date:	29-OCT-2001
Revision date:	
Date of last Update:	29-OCT-2001

Number of Pages:	27

Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

I U C L I D

D a t a S e t

Existing Chemical	ID: 102-27-2
CAS No.	102-27-2
EINECS Name	N-ethyl-m-toluidine
EINECS No.	203-019-4
Molecular Weight	135.2
Molecular Formula	C9H13N

Producer Related Part
Company:
Creation date: 15-JUL-1999

Substance Related Part
Company:
Creation date: 15-JUL-1999

Memo: Bayer Corporation

Printing date: 29-OCT-2001
Revision date:
Date of last Update: 29-OCT-2001

Number of Pages: 21

Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 7
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 OECD and Company Information

Type: lead organisation
Name: American Chemistry Council (formerly Chemical Manufacturers Association), Monocyclic Aromatic Amines and Nitro Aromatics (MAANA) HPV Panel
Street: 1300 Wilson Boulevard
Town: 22209 Arlington, VA
Country: United States

21-AUG-2001

Type: cooperating company
Name: Albemarle Corporation
Country: United States

25-SEP-2001

Type: cooperating company
Name: Bayer Corporation
Country: United States

25-SEP-2001

Type: cooperating company
Name: Buffalo Color
Country: United States

25-SEP-2001

Type: cooperating company
Name: First Chemical Corporation
Country: United States

25-SEP-2001

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information
-

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms
-

1.3 Impurities
-

1.4 Additives
-

1.5 Quantity
-

1.6.1 Labelling
-

1.6.2 Classification
-

1.7 Use Pattern
-

1.7.1 Technology Production/Use
-

1.8 Occupational Exposure Limit Values
-

1.9 Source of Exposure
-

1.10.1 Recommendations/Precautionary Measures
-

1.10.2 Emergency Measures
-

1.11 Packaging
-

1.12 Possib. of Rendering Subst. Harmless
-

1.13 Statements Concerning Waste
-

1.14.1 Water Pollution
-

1.14.2 Major Accident Hazards
-

1.14.3 Air Pollution
-

1.15 Additional Remarks
-

1.16 Last Literature Search
-

1.17 Reviews
-

1.18 Listings e.g. Chemical Inventories
-

2.1 Melting Point

Value: 8.7 degree C
Method: other: (calculated) MPBPWIN (v1.31)
Year: 1999
Testsubstance: other TS: molecular structure
Result: Melting Point: 9.63 deg C (Adapted Joback Method)
Melting Point: 7.84 deg C (Gold and Ogle Method)
Mean Melt Pt : 8.74 deg C (Joback; Gold, Ogle Methods)
Selected MP: 8.74 deg C (Mean Value)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
19-JUN-2001 (1)

2.2 Boiling Point

Value: 221 degree C
Method: other: Handbook value
Testsubstance: other TS: N-ethyl-m-toluidine; purity not stated
Reliability: (2) valid with restrictions
Data from Handbook or collection of data
Flag: Critical study for SIDS endpoint
19-JUN-2001 (2)

2.3 Density

Type: density
Value: ca. .945 g/cm3 at 20 degree C
Testsubstance: other TS: N-ethyl-m-toluidine; purity not stated
Flag: Critical study for SIDS endpoint
09-APR-2001 (3)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: .17 hPa (0.125 mm) at 25 degree C
Method: other (calculated): MPBPWIN (v1.40)
Testsubstance: other TS: molecular structure
Result: Vapor Pressure Estimations (25 deg C):
(Using BP: 221.00 deg C (estimated))
(MP not used for liquids)
VP: 0.133 mm Hg (Antoine Method)
VP: 0.116 mm Hg (Modified Grain Method)
VP: 0.196 mm Hg (Mackay Method)
Selected VP: 0.125 mm Hg (Mean of Antoine & Grain methods)
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint

16-AUG-2001 (1)

Value: 1.33 hPa (1.0 mm) at 54 degree C
Testsubstance: other TS: N-ethyl-m-toluidine; purity not stated
Flag: Critical study for SIDS endpoint
16-AUG-2001 (3)

2.5 Partition Coefficient

log Pow: 2.662
Method: other (calculated): KOWWIN Program (v1.65)
Year: 1999
GLP: no
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
16-AUG-2001 (1)

log Pow: 2.7
Method: other (calculated): A. Leo, CLOPG-3.54 MedChem Software 1989. Daylight, Chemical Information Systems, Claremont, CA 91711, USA
Year:
GLP: no
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
16-AUG-2001 (4)

2.6.1 Water Solubility

Value: 1131 mg/l at 20 degree C
Method: OECD Guide-line 105 "Water Solubility"
GLP: yes
Testsubstance: other TS: N-ethyl-m-toluidine; purity = 99.223% by GC (1992-09-14)
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
16-AUG-2001 (5)

2.6.2 Surface Tension
-

2.7 Flash Point

Value: ca. 93 degree C
Type:
Method: other: DIN 51758
Year:
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
16-AUG-2001 (3)

2.8 Auto Flammability
-

2.9 Flammability
-

2.10 Explosive Properties
-

2.11 Oxidizing Properties

Result: maximum burning rate equal or higher than reference mixture
16-AUG-2001

2.12 Additional Remarks
-

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1560000 molecule/cm3
Rate constant: ca. .0000000001203522 cm3/(molecule * sec)
Degradation: 50 % after 1.1 hour(s)
Method: other (calculated): AOP v1.89
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
16-AUG-2001 (1)

3.1.2 Stability in Water

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 106-49-0; 121-69-7.

3.1.3 Stability in Soil
-

3.2 Monitoring Data (Environment)
-

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: air, water, soil, sediment
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: (calculation) Level III Fugacity Model
Year: 1999
Result:

Media	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	0.176	2.13	1000	5.67e-012
Water	32.5	900	1000	1.31e-010
Soil	67	900	1000	6.27e-010
Sediment	0.305	3.6e+003	0	1.12e-010

Persistence Time: 595 hr
Reaction Time: 747 hr
Advection Time: 2.92e+003 hr
Percent Reacted: 79.6
Percent Advected: 20.4
Reliability: (2) valid with restrictions
Accepted calculation method

Flag: Critical study for SIDS endpoint
16-AUG-2001 (1)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge, adapted
Degradation: 0 % after 20 day
Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year: 1976 GLP: no
Test substance: other TS: other TS: N-ethyl-m-toluidine; purity =99.5 %
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
09-APR-2001

3.6 BOD5, COD or BOD5/COD Ratio
-

3.7 Bioaccumulation

Species: other
Exposure period:
Concentration:
BCF: 22.36
Elimination:
Method: other: BCF Program (v2.13)
Year: GLP:
Test substance: other TS: molecular structure
Result: Log Kow (estimated) : 2.66
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 2.66

Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70

Estimated Log BCF = 1.350 (BCF = 22.36)
Reliability: (2) valid with restrictions
Accepted calculation method
16-AUG-2001 (1)

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: yes
LC50: 49.5
Method: EPA OPP 72-1
Year: 1981 GLP: no data
Test substance: other TS: N-ethyl-m-toluidine; purity not stated
Reliability: (1) valid without restriction
Guideline study
Flag: Critical study for SIDS endpoint
16-AUG-2001 (6)

Type: static
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
LC0: 50
LC100: 100
Method: other: Determination of the acute effects of substances on fish.“Fish test” research group in the "Detergents" advisory committee (10/15/73)
Year: 1976 GLP: no
Test substance: other TS: N-ethyl-m-toluidine; purity = 99.5 %
Remark: range finding test
Reliability: (2) valid with restrictions
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
25-SEP-2001 (7)

Type: other: calculation
Species: other: Fish
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
LC50: 24.022
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Remark: ECOSAR Class: Neutral Organics
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
16-AUG-2001 (1)

Type: other: calculation
Species: other: Fish
Exposure period: 14 day
Unit: mg/l Analytical monitoring: no
LC50: 48.323
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Remark: ECOSAR Class: Neutral Organics
Reliability: (2) valid with restrictions
Accepted calculation method
16-AUG-2001 (1)

4.2 Acute Toxicity to Aquatic Invertebrates

Type: other: calculation
Species: Daphnia sp. (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 26.941
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
19-JUN-2001 (1)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: other algae: Green Algae
Endpoint: other: calculation
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 17.495
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
19-JUN-2001 (1)

4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: Pseudomonas fluorescens (Bacteria)
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring: no
EC0: 1000
Method: other: Deterimination of the harmful biological effects of toxic sewage on bacteria. DEV, L 8 (1968) modified
Year: 1976 GLP: no
Test substance: other TS: N-ethyl-m-toluidine; purity = 99.5 %
09-APR-2001 (7)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish
-

4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms
-

4.6.2 Toxicity to Terrestrial Plants
-

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species
-

4.7 Biological Effects Monitoring
-

4.8 Biotransformation and Kinetics
-

4.9 Additional Remarks
-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type:	LD50
Species:	rat
Strain:	Sprague-Dawley
Sex:	male/female
Number of Animals:	
Vehicle:	other: corn oil
Value:	787 mg/kg bw
Method:	other: USEPA TSCA Health Effects Testing Guidelines, 40 CFR 798.1175, "Acute Oral Toxicity", 1992.
Year:	1992 GLP: yes
Test substance:	other TS: N-ethyl-m-toluidine; purity = 98.67%
Method:	Animals used: 5 per sex/dose group; Doses were: 100, 500, 750, 1000 mg/kg bw
Remark:	Test material analysis not done under GLP
Result:	LD 50 (95% CI)= 585-1058 mg/kg bw
Reliability:	(1) valid without restriction GLP guideline study
Flag:	Critical study for SIDS endpoint

25-SEP-2001 (8)

Type:	LD50
Species:	rat
Strain:	Wistar
Sex:	male/female
Number of Animals:	
Vehicle:	other: none
Value:	650 mg/kg bw
Method:	Directive 84/449/EEC, B.1 "Acute toxicity (oral)"
Year:	1980 GLP: no data
Test substance:	other TS: N-ethyl-m-toluidine; purity not stated
Method:	5 rats/sex/dose, single application by gavage; 6 doses: 0.5, 0.6,0.7, 0.8, 1.0, 1.2 ml/kg bw; observation time 14 d, statistical evaluation
Remark:	0.5 ml was accepted without impairment, no mortality; 0.6,0.7, 0.8, 1.0, 1.2 ml/kg bw: all rats displayed slight symptoms of intoxication from 15 min. post application until death including cyanotic appearance and reduced general condition, females suffered additionally from decrease in body weight. Death occurred from 4 hours until the 4th day post treatment: 3/10, 7/10, 7/10, 9/10, 10/10
Reliability:	(1) valid without restriction Guideline study
Flag:	Critical study for SIDS endpoint

17-AUG-2001 (9)

5.1.2 Acute Inhalation Toxicity

Type:	LC50
Species:	rat
Strain:	no data
Sex:	no data
Number of Animals:	
Vehicle:	no data
Exposure time:	4 hour(s)
Value:	2.4 mg/l
Method:	other: no data
Year:	GLP: no data
Test substance:	other TS: N-ethyl-m-toluidine; purity not stated
Remark:	Toxic effects observed include labored breathing, decreased muscle tone, cyanosis, and loss of reflexes.

25-SEP-2001 (10)

5.1.3 Acute Dermal Toxicity

Type:	LD50
Species:	rabbit
Strain:	New Zealand white
Sex:	male/female
Number of Animals:	10
Vehicle:	
Value:	> 2000 mg/kg bw
Method:	other: USEPA TSCA Health Effects Testing Guidelines, 40CFR 798.1100, "Acute Dermal Toxicity", 1992
Year:	1992 GLP: yes
Test substance:	other TS: N-ethyl-m-toluidine; purity > 97%
Remark:	Animals used: 5/sex/dose group
Reliability:	(1) valid without restriction GLP guideline study
Flag:	Critical study for SIDS endpoint

25-SEP-2001 (11)

5.1.4 Acute Toxicity, other Routes

-

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species:	rabbit	
Concentration:	undiluted	
Exposure:	Occlusive	
Exposure Time:	4	hour(s)
Number of Animals:	6	
PDII:	.7	
Result:	slightly irritating	
EC classificat.:	not irritating	
Method:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"	
Year:	1992	GLP: yes
Test substance:	other TS: N-ethyl-m-toluidine; purity > 97%	
Remark:	3 male and 3 female New Zealand white rabbits were exposed; all animals were scored after unwrapping and at day 7. PDII = 0.7/8 Test material analysis was not done under GLP.	
Reliability:	(1) valid without restriction GLP guideline study	
Flag:	Critical study for SIDS endpoint	

25-SEP-2001 (12)

Species:	rabbit	
Concentration:		
Exposure:		
Exposure Time:		
Number of Animals:		
PDII:		
Result:	slightly irritating	
EC classificat.:		
Method:		
Year:		GLP:
Test substance:	other TS: N-ethyl-m-toluidine; purity not stated	
Remark:	exposure period: 24 hours	
Flag:	Critical study for SIDS endpoint	

17-AUG-2001 (7)

5.2.2 Eye Irritation

Species: rabbit
Concentration: undiluted
Dose: .1 ml
Exposure Time:
Comment: not rinsed
Number of Animals: 6
Result: not irritating
EC classificat.: not irritating
Method: EPA OTS 798.4500
Year: 1992 GLP: yes
Test substance: other TS: N-ethyl-m-toluidine; purity = 98.67%
Remark: 6 female New Zealand white rabbits were exposed. Test material analysis was not done under GLP.
Result: Maximum score of 9.8/110 at the 24 hour scoring interval; all signs of irritation had cleared by 72 hours after dosing.
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
25-SEP-2001 (13)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: slightly irritating
EC classificat.:
Method:
Year: GLP:
Test substance: other TS: N-ethyl-m-toluidine; purity not stated
Flag: Critical study for SIDS endpoint
17-AUG-2001 (7)

5.3 Sensitization

Type: Buehler Test
Species: rabbit
Concentration: Induction undiluted
Challenge 50 %
Number of Animals:
Vehicle: other: acetone
Result: not sensitizing
Classification: not sensitizing
Method: other: according to Ritz, H.L., and Buehler, E.V., Current Concepts in Cutaneous toxicity, eds. Drill, V.A., and Lazar T. (Academic Press, 1980), pp. 25-40
Year: 1980 GLP: yes
Test substance: other TS: N-ethyl-m-toluidine; purity = 98.115

Remark: 20 test animals (10 male, 10 female) and 10 naive controls (5 male, 5 female);
Induction and challenge applications were dermal using 0.3 ml test substance in each Hilltop chamber;
Naive control was treated with 50% test material in acetone; controls were common to this study and one other. Test material analysis was not done under GLP.

Result:

Response:	Test animals	Naive controls
Grade 1	0/20	2/10
Grade +/-	16/20	8/10
Grade 0	4/20	0/10

At the time of the 24 hr reading, residual Neet (dipilatory) was noted on several of the dosing sites in the naive control group (including 2 animals with a grade 1 result). The Neet may have created artificial irritaion at the sites. The irritation in these animals was reduced to a grade of +/- by the 48 hr reading. The interpretation of the primary challenge data was not compromised by this occurrence. The responses produced in the test group were essentially comparable to the naive group, indicating that sensitization had not been induced.

Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
25-SEP-2001 (14)

5.4 Repeated Dose Toxicity

Species: rat Sex: male/female
Strain: Sprague-Dawley
Route of admin.: inhalation
Exposure period: 2 weeks
Frequency of treatment: 6 hr/day, 5 days/week
Post. obs. period: 2 weeks, control and high exposure groups
Doses: 5.6, 32.8, 67.6 ppm
Control Group: yes, concurrent no treatment
NOAEL: = 5.6 ppm
Method: OECD Guide-line 412 "Repeated Dose Inhalation Toxicity: 28-day or 14-day Study"
Year: 1981 GLP: yes
Test substance: other TS: N-ethyl-m-toluidine; purity = 98.68%
Remark: Test material analysis not done under GLP. TSCA Substantial Risk notice.
Result: There were no deaths, and no changes in body weights, food consumption, clinical observations, or clinical chemistry. Methemoglobinemia was significantly increased across all exposure groups at both terminal and recovery necropsies in both sexes. Enlarged spleens, increased production of red cells in the spleen, bone marrow, and liver, and other hematology changes were consistent with induction of hemolytic anemia. Kidney effects were considered secondary to hemolytic anemia. This condition was not completely

reversed at the end of the 14 day recovery period. A "no effect level" was not established under the conditions of this study. However, the lowest exposure level of 5.6 ppm was considered a "no adverse effect level" because the increase in methemoglobin was not accompanied by adverse histopathology or clinical signs.
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
25-SEP-2001 (15)

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 106-49-0; 108-44-1; 121-69-7; 91-66-7.

5.5 Genetic Toxicity 'in Vitro'

Type: Bacterial reverse mutation assay
System of testing: Salmonella strains TA98, TA100, TA1535, TA1537,
Concentration: 100, 250, 500, 1000, 2500, 5000 ug/plate
Cytotoxic Conc.: 3330 ug/plate - S9 in TA100;
2500ug/plate - S9 in other strains
Metabolic activation: without
Result: negative
Method: OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year: 1983 GLP: yes
Test substance: other TS: N-ethyl-m-toluidine; purity = 98.115%
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
17-AUG-2001 (16)

Type: Bacterial reverse mutation assay
System of testing: Salmonella strains TA98, TA100, TA1535, TA1537,
Concentration: 100, 250, 500, 1000, 2500, 5000 ug/plate
Cytotoxic Conc.: 3330 ug/plate + S9 in TA100;
5000ug/plate + S9 in other strains
Metabolic activation: with
Result: positive
Method: OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year: 1983 GLP: yes
Test substance: other TS: N-ethyl-m-toluidine; purity = 98.115%
Remark: Test material analysis not done under GLP. The only deviation from guidelines was lack of a confirmatory assay. However, a separate study was done to confirm positive results in TA98 with activation (ChemFirst Study No. 18688-0-401SC)
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
17-AUG-2001 (16)

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537
Concentration: up to 200 µg/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: positive
Method: Directive 84/449/EEC, B.14 "Other effects - Mutagenicity (Salmonella typhimurium - reverse mutation assay)"
Year: 1994 GLP: yes
Test substance: other TS: N-ethyl-m-toluidine; purity = 99.223 %
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
17-AUG-2001 (17)

Type: Escherichia coli reverse mutation assay
System of testing: E. coli strain WP2uvrA
Concentration: 100, 250, 500, 1000, 2500, 5000 ug/plate
Cytotoxic Conc.: 5000ug/plate +/- S9
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 472 "Genetic Toxicology: Escherichia coli Reverse Mutation Assay"
Year: 1983 GLP: yes
Test substance: other TS: N-ethyl-m-toluidine; purity = 98.115%
Remark: Test material analysis not done under GLP.
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
17-AUG-2001 (16)

5.6 Genetic Toxicity 'in Vivo'

-

5.7 Carcinogenicity

-

5.8 Toxicity to Reproduction

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 106-49-0; 108-44-1; 121-69-7.

5.9 Developmental Toxicity/Teratogenicity

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 121-69-7; 91-66-7.

5.10 Other Relevant Information
-

5.11 Experience with Human Exposure
-

(1) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510.

(2) CRC Handbook of Chemistry and Physics. 80th edition (1999-2000) David R. Lide, ed. CRC Press, New York. p3-23 No. 747.

(3) Safety Data Sheet Bayer AG, 28.03.1989

(4) Calculation Bayer AG, UWS-Produktsicherheit

(5) Bayer AG study (1992-10-08)

(6) L.T. Brooke et al, Acute Toxicities of Organic Chemicals to Fathead Minnows(Pimephales Promelas) vol.1, Center for Lake Superior Environment Studies, Univ. of Wisconsin, Superior, WI (1984).

(7) Bayer AG data

(8) ChemFirst Study No. L08604-37

(9) E. Löser, Bayer AG data, N-Äthyl-m-toluidin rein: untersuchungen zur akuten Toxizität an männlichen und weiblichen Wistar Ratten, 25. Nov.1980

(10) Safety Data Sheet, DuPont de Nemours and Company, N-ethyl-m-toluidine, MSDS Number DU003000_00, revised 9/7/93.

(11) ChemFirst Study No. L08583-7

(12) ChemFirst Study No. L08583-8

(13) ChemFirst Study No. L08604-36

(14) ChemFirst Study No. 95-8607-21

(15) ChemFirst Study No.L08689-2

(16) ChemFirst Study No. 16861-0-409 (1995)

(17) Bayer AG, Report No. 23463, 08.11.1994

7.1 End Point Summary

-

7.2 Hazard Summary

-

7.3 Risk Assessment

-

1.0.1 OECD and Company Information

Type: lead organisation
Name: American Chemistry Council (formerly Chemical Manufacturers Association), Monocyclic Aromatic Amines and Nitro Aromatics (MAANA) HPV Panel
Street: 1300 Wilson Boulevard
Town: 22209 Arlington, VA
Country: United States

17-AUG-2001

Type: cooperating company
Name: Albemarle Corpoiration
Country: United States

24-SEP-2001

Type: cooperating company
Name: Bayer Corporation
Country: United States

24-SEP-2001

Type: cooperating company
Name: Buffalo Color Corporation
Country: United States

24-SEP-2001

Type: cooperating company
Name: ChemFirst Inc
Country: United States

24-SEP-2001

1.0.2 Location of Production Site
-

1.0.3 Identity of Recipients
-

1.1 General Substance Information

Substance type: organic
Physical status: liquid
21-OCT-1999

1.1.0 Details on Template
-

1.1.1 Spectra
-

1.2 Synonyms

Benzenamine, N-ethyl-
21-OCT-1999

1.3 Impurities
-

1.4 Additives
-

1.5 Quantity
-

1.6.1 Labelling
-

1.6.2 Classification
-

1.7 Use Pattern

Type: type
Category: Use in closed system
21-OCT-1999

Type: industrial
Category: Chemical industry: used in synthesis
21-OCT-1999

Type: use
Category: Intermediates
21-OCT-1999

1.7.1 Technology Production/Use
-

1.8 Occupational Exposure Limit Values
-

1.9 Source of Exposure
-

1.10.1 Recommendations/Precautionary Measures
-

1.10.2 Emergency Measures
-

1.11 Packaging
-

1.12 Possib. of Rendering Subst. Harmless
-

1.13 Statements Concerning Waste
-

1.14.1 Water Pollution
-

1.14.2 Major Accident Hazards
-

1.14.3 Air Pollution
-

1.15 Additional Remarks
-

1.16 Last Literature Search
-

1.17 Reviews
-

1.18 Listings e.g. Chemical Inventories
-

2.1 Melting Point

Value:	-64 degree C	
Method:	other	
GLP:	no data	
Testsubstance:	other TS: N-ethylaniline; purity not stated	
Reliability:	(2) valid with restrictions Handbook value	
Flag:	Critical study for SIDS endpoint	
21-AUG-2001		(1)

Value:	-63.5 degree C	
Method:	other:	
GLP:	no data	
Testsubstance:	other TS: N-ethylaniline; purity not stated	
Reliability:	(2) valid with restrictions Handbook value	
Flag:	Critical study for SIDS endpoint	
21-AUG-2001		(2)

2.2 Boiling Point

Value:	203 degree C at 1013 hPa	
Decomposition:	no	
Method:	other:	
GLP:	no data	
Testsubstance:	other TS: N-ethylaniline; purity not stated	
Reliability:	(2) valid with restrictions Handbook value	
Flag:	Critical study for SIDS endpoint	
21-AUG-2001		(2)

Value:	204.5 degree C at 1013 hPa	
Decomposition:	no	
Method:	other	
GLP:	no data	
Testsubstance:	other TS: N-ethylaniline; purity not stated	
Reliability:	(2) valid with restrictions Handbook value	
Flag:	Critical study for SIDS endpoint	
21-AUG-2001		(3)

Value:	207 degree C	
Method:	other	
GLP:	no data	
Testsubstance:	other TS: N-ethylaniline; purity not stated	
Reliability:	(2) valid with restrictions Handbook value	
Flag:	Critical study for SIDS endpoint	
21-AUG-2001		(1)

2.3 Density

Type:
Value: .9625 at 20 degree C
Method: other:
GLP: no data
Testsubstance: other TS: N-ethylaniline; purity not stated
Reliability: (2) valid with restrictions
Handbook value
Flag: Critical study for SIDS endpoint
21-AUG-2001 (2) (1)

2.3.1 Granulometry
-

2.4 Vapour Pressure

Value: = .4 hPa at 20 degree C
Testsubstance: other TS: N-ethylaniline; purity not stated
Reliability: (2) valid with restrictions
Handbook value
Flag: Critical study for SIDS endpoint
21-AUG-2001 (1)

Value: 1 hPa at 38 degree C
Method: other (measured):
GLP: no data
Testsubstance: other TS: N-ethylaniline; purity not stated
Reliability: (2) valid with restrictions
Handbook value
Flag: Critical study for SIDS endpoint
21-AUG-2001 (4)

Value: 1.9 at 50 degree C
Method: other (measured)
Testsubstance: other TS: N-ethylaniline; purity not stated
Reliability: (2) valid with restrictions
Handbook value
Flag: Critical study for SIDS endpoint
21-AUG-2001 (1)

2.5 Partition Coefficient

log Pow: 1.92 at 25 degree C
Method: other (measured): OECD Chemicals Testing Programme Ecotoxicology Group
Year: 1979
GLP: yes
Testsubstance: other TS: N-ethylaniline; purity not stated
Remark: Octanol/Water partition coeffiecient P= 82.30
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
21-AUG-2001 (5)

log Pow: 2.26 at 25 degree C
Method: other (measured): shake-flask method according to Fujita t, Iwasa J, Hansch C. 1964. J. Am. Chem. Soc. 86:5175.
Year:
GLP: no data
Testsubstance: other TS: N-ethylaniline; purity not noted
Remark: Method of equlibration: Shake-flask
Analytical method: absorption spectrophotometry
Aqueous phase: octanol-saturated water
Phase analyzed: aqueous
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
21-AUG-2001 (6) (7)

log Pow: 2.16
Method: other (measured)
Year:
GLP: no
Testsubstance: other TS: N-ethylaniline; purity not stated
Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
21-AUG-2001 (7) (8)

log Pow: 2.114
Method: other (calculated): KOWWIN Program (v1.65)
Year:
Testsubstance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
21-AUG-2001 (9)

2.6.1 Water Solubility

Value:	ca. 2700 mg/l at 20 degree C
Qualitative:	soluble (1000-10000 mg/L)
pH:	1
Method:	other
Testsubstance:	other TS: N-ethylaniline; purity not stated
Reliability:	(2) valid with restrictions Handbook value
Flag:	Critical study for SIDS endpoint

21-AUG-2001 (1)

2.6.2 Surface Tension
-

2.7 Flash Point
-

2.8 Auto Flammability
-

2.9 Flammability
-

2.10 Explosive Properties
-

2.11 Oxidizing Properties
-

2.12 Additional Remarks
-

3.1.1 Photodegradation

Type: air
INDIRECT PHOTOLYSIS
Sensitizer: OH
Conc. of sens.: 1560000 molecule/cm3
Rate constant: = .0000000000515114 cm3/(molecule * sec)
Degradation: 50 % after 2.5 hour(s)
Method: other (calculated): AOP v1.89
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
21-AUG-2001 (9)

3.1.2 Stability in Water

Type: abiotic
t1/2 pH : 1.1 day
Method: other: careful sampling of Rhine river water at Lobith and 24.5 hours later at Gorinchem as carried out by GC-MS analysis of concentrates prepared by closed-loop gas-stripping and XAD adsorption techniques.
Year: GLP: no
Test substance: other TS: N-ethylaniline; 97.5% purity
Remark: The half life is much longer in stagnant waters or groundwaters due to limited volatilization, aerobic biodegradation and photochemical decomposition.
Test condition: Under field conditions, in running water, the half life of N-ethylaniline is estimated to be 1.1. days.
21-AUG-2001 (10)

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 106-49-0; 121-69-7.

3.1.3 Stability in Soil
-

3.2 Monitoring Data (Environment)

Type of measurement: other: field study
Medium: surface water
Method: On July 16, 1979 a careful sampling of Rhine river water at Lobith and 24.5 hours later at Gorinchem as carried out by GC-MS analysis of concentrates prepared by closed-loop gas-stripping and XAD adsorption techniques.
Concentration .3 - µg/l
Result: Relevant concentration at Lobith was 0.3 ug/l and estmated half-life was 1.1 days.
19-JUN-2001 (10)

3.3.1 Transport between Environmental Compartments

Type: fugacity model level III
Media: other: Air Water Soil Sediment
Air (Level I):
Water (Level I):
Soil (Level I):
Biota (L.II/III):
Soil (L.II/III):
Method: other: (calculation) EPIWIN Level III Fugacity Model
Year: 1999
Result:

Media	Distribution (percent)	Half-Life (hr)	Emissions (kg/hr)	Fugacity (atm)
Air	0.88	4.98	1000	1.46e-011
Water	42.2	360	1000	2.34e-010
Soil	56.8	360	1000	2.03e-009
Sediment	0.149	1.44e+003	0	1.7 e-010

Persistence Time: 275 hr
Reaction Time: 320 hr
Advection Time: 1.96e+003 hr
Percent Reacted: 86
Percent Advected: 14
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
21-AUG-2001 (9)

3.3.2 Distribution
-

3.4 Mode of Degradation in Actual Use
-

3.5 Biodegradation

Type: aerobic
Inoculum:
Degradation: 0 % after 28 day
Method: OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year: 1977 GLP: no data
Test substance: other TS: N-ethylaniline; purity not noted
Reliability: (1) valid without restriction
Guideline Study
Flag: Critical study for SIDS endpoint
24-SEP-2001 (11)

Type: aerobic
Inoculum:
Concentration: 19.1 mg/l related to DOC (Dissolved Organic Carbon)
23.7 mg/l related to Test substance
Degradation: 97 % after 14 day
Method: ISO 7827 "Evaluation in an aqueous medium of the 'ultimate' aerobic biodegradability of organic compounds - method by anlaysis of dissolved organic carbon (DOC)"
Year: GLP: no data
Test substance: other TS: N-ethylaniline; purity not noted
Remark: BOD = 0.048 g/g
BOD5/COD = 64.3%
Reliability: (1) valid without restriction
Meets National standards method (AFNOR/DIN)
Flag: Critical study for SIDS endpoint
24-SEP-2001 (12)

3.6 BOD5, COD or BOD5/COD Ratio

Method: other: Modified OECD Screening Test, ISO 7827

Result: 19.1 mg DOC of N-ethylaniline (23.7 mg) eliminated in 14 days to an extent of 97% (BOD5/COD = 64.3%)
BOD = 0.048 g/g
Reliability: (2) valid with restrictions
Guideline study with acceptable restrictions
21-AUG-2001 (13)

3.7 Bioaccumulation

Species:
Exposure period:
Concentration:
BCF: 9.19
Elimination:
Method: other: BCF Program (v2.13) no
Year: GLP:
Test substance: other TS: molecular structure
Remark: Log Kow (estimated) : 2.11
Log Kow (experimental): 2.16
Log Kow used by BCF estimates: 2.16

Equation Used to Make BCF estimate:
Log BCF = 0.77 log Kow - 0.70

Estimated Log BCF = 0.963 (BCF = 9.188)
Reliability: (2) valid with restrictions
Accepted calculation method
21-AUG-2001 (9)

3.8 Additional Remarks
-

AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type:			
Species:	Oryzias latipes (Fish, fresh water)		
Exposure period:	48 hour(s)		
Unit:	mg/l	Analytical monitoring:	no data
LC50:	= 33		
Method:	other: other: according to Japan Industrial Standards		
Year:	1971	GLP:	no data
Test substance:	other TS: N-ethylaniline; purity not noted		
Remark:	Substances which were difficult to dissolve in water were dissolved in 1 ml. of ethanol then diluted with water.		
Result:	LC50 (24 hr) = 71 mg/l		
Reliability:	(1) valid without restriction Meets National standards method (AFNOR/DIN)		
Flag:	Critical study for SIDS endpoint		
21-AUG-2001			(14)

Type:	other: calculation		
Species:	other: Fish		
Exposure period:	96 hour(s)		
Unit:	mg/l	Analytical monitoring:	no
LC50:	70.802		
Method:	other: ECOSAR v0.99e		
Year:	1999	GLP:	no
Test substance:	other TS: molecular structure		
Reliability:	(2) valid with restrictions Accepted calculation method		
Flag:	Critical study for SIDS endpoint		
21-AUG-2001			(9)

Type:			
Species:	Brachydanio rerio (Fish, fresh water)		
Exposure period:	96 hour(s)		
Unit:	mg/l	Analytical monitoring:	no data
LC0:	= 50		
Method:	other: No data		
Year:		GLP:	no data
Test substance:	no data		
19-JUN-2001			(15)

Type:	other: calculation		
Species:	other: Fish		
Exposure period:	14 day		
Unit:	mg/l	Analytical monitoring:	no
LC50:	130.507		
Method:	other: ECOSAR v0.99e		
Year:	1999	GLP:	no
Test substance:	other TS: molecular structure		
Reliability:	(2) valid with restrictions		
24-APR-2001			(9)

Type:
Species: Leuciscus idus (Fish, fresh water)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50: 10
Method: other: No data
Year: GLP: yes
Test substance:
24-APR-2001 (16)

4.2 Acute Toxicity to Aquatic Invertebrates

Type: other: calculation
Species: Daphnia sp. (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 76.444
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
21-AUG-2001 (9)

Type:
Species: Daphnia magna (Crustacea)
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no data
EC0: 6.3
EC50: 18
EC100: 50
Method: other: no data
Year: GLP: yes
Test substance: no data
Flag: Critical study for SIDS endpoint
21-AUG-2001 (16)

Type:
Species: other: Tetrahymena pyriformis
Exposure period: 24 hour(s)
Unit: mg/l Analytical monitoring: yes
EC50: 160
Method:
Year: GLP: yes
Test substance: no data
Method: T. pyriformis was pre-cultured at 30 degree C for 24 hr. Concentration for stock solution was 1.8 in 10 ml 2% protease peptone. Slightly soluble chemicals were dissolved in dimethylsulfoxide (DMSO). Stock solutions were inoculated with 0.2 ml of T. pyriformis and cultivated at 30 degree C for 24 hr without agitation. Cells were then counted by Coulter Counter and microscope (correlation coefficient was 0.998, n=32)

Reliability: (2) valid with restrictions
Meets generally accepted scientific standards, well documented and acceptable for assessment
Flag: Critical study for SIDS endpoint
28-SEP-2001 (18)

Type:
Species: other: Chaetogammarus marinus
Exposure period: 90 hour(s)
Unit: mg/l Analytical monitoring: no data
EC50: 44
Method: other: no data
Year: GLP: no data
Test substance: no data
24-APR-2001 (17)

Type: other: calculation
Species: Mysidopsis bahia (Crustacea)
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 18.877
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
24-APR-2001 (9)

Type: other: calculation
Species: Daphnia sp. (Crustacea)
Exposure period: 16 day
Unit: mg/l Analytical monitoring: no
EC50: 4.114
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
24-APR-2001 (9)

Type:
Species: other: Tubitex species
Exposure period: 48 hour(s)
Unit: mg/l Analytical monitoring: no data
LC50 : 160
Method: other: no data
Year: GLP: no data
Test substance: no data
Result: LC50 (24 hr) = 470 mg/l
09-AUG-2000 (19)

4.3 Toxicity to Aquatic Plants e.g. Algae

Species: other algae: green algae
Endpoint: growth rate
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no
EC50: 48.094
ChV : 5.125
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
Flag: Critical study for SIDS endpoint
21-AUG-2001 (9)

Species: Scenedesmus subspicatus (Algae)
Endpoint:
Exposure period: 96 hour(s)
Unit: mg/l Analytical monitoring: no data
EC10: 17
EC50: 98
Method: other: no data
Year: GLP: no data
Test substance: no data
Flag: Critical study for SIDS endpoint
21-AUG-2001 (20) (16)

Species: Agmenellum quadruplicatum (Algae)
Endpoint: other: algal lawn assay (growth inhibition
Exposure period: 7 day
Unit: Analytical monitoring: no
Method:
Year: GLP:
Test substance: other TS: N-ethylaniline; purity not noted
Method: Algal lawns were initially seeded with 1.0 x 10e+5 cells/ml in 1% agarized (Difco 0140) medium. The test chemical was absorbed onto antibiotic sensitivity disks (12.7 mm; Schleicher and Schuell, No. 740-E) which were placed directly onto the agar surface. The petri dish cultures were sealed with Scotch Tape and incubated in light from a tungsten lamp for 3-7 days at 28-30 degree C. Zone of inhibition was measured from the edge of the disk in mm. The radius of growth inhibition around the disk was judged visually and microscopically.
Result:

Concentration (ug/disk)	zone of inhibition (mm)
0	0
1	0
10	0
100	0
500	2
1000	10

0 indicates no inhibition,36 indicates complete inhibition.
No inhibittion was noted with ethanol controls.

LC50 >1000 ug/disk
Reliability: (3) invalid
Not a Guideline method
21-AUG-2001 (21)

4.4 Toxicity to Microorganisms e.g. Bacteria
-

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

Species: other
Endpoint: other
Exposure period: 30 day
Unit: mg/l Analytical monitoring: no
ChV : 9.284
Method: other: ECOSAR v0.99e
Year: 1999 GLP: no
Test substance: other TS: molecular structure
Reliability: (2) valid with restrictions
Accepted calculation method
21-AUG-2001 (9)

4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

Type:	other: calculation
Species:	Eisenia fetida (Worm (Annelida), soil dwelling)
Endpoint:	other
Exposure period:	14 day
Unit:	other: ppm
LC50:	689.546
Method:	other: ECOSAR v0.99e
Year:	1999 GLP: no
Test substance:	other TS: molecular structure
Remark:	Chemical may not be soluble enough to measure this predicted effect.
Reliability:	(2) valid with restrictions Accepted calculation method

21-AUG-2001 (9)

4.6.2 Toxicity to Terrestrial Plants
-

4.6.3 Toxicity to other Non-Mamm. Terrestrial Species
-

4.7 Biological Effects Monitoring
-

4.8 Biotransformation and Kinetics
-

4.9 Additional Remarks
-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Strain: Sprague-Dawley
Sex: male/female
Number of Animals: 10
Vehicle: other: corn oil
Value: = 478 mg/kg bw
Method: other: USEPA TSCA Health Effects Testing Guidelines, 40 CFR 798.1175, "Acute Oral Toxicity"
Year: 1992 GLP: yes
Test substance: other TS: N-Ethylaniline, purity 99.19%
Remark: Test material analysis not done under GLP
Result: 95% CI = 308-741 mg/kg bw
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
21-AUG-2001 (22)

Type: LD50
Species: rat
Strain: Sprague-Dawley
Sex: male/female
Number of Animals: 10
Vehicle: other: undiluted
Value: 332.2 - 401.6 mg/kg bw
Method: other: OECD Acute Oral Toxicity Protocol - modified
Year: GLP: yes
Test substance: other TS:Commercial purity: 97.5%
Remark: Undiluted N-ethylaniline was administered in a single dose at 275.0 mg/kg, 307.0 mg/kg, 342.0 mg/kg, 381.0 mg/kg, and 425.0 mg/kg to groups of five female and five male Sprague-Dawley rats. Animals were fasted overnight. Where possible, the volume of dosing solution did not exceed 5 ml. per animal. Pale skin was noted at the 275.0 and 342.0 mg/kg doses. Ataxia, pale skin, and deaths were noted at the 307.0 and 381.0 doses. Ataxia and death were noted at 425.0 mg/kg. Lungs which were dark in color were observed at necropsy.
LD50 calculated according to Finney DJ. "Statistical Methods in Biological Assay. 2nd ed. London:Griffin Press. 1971.
Result:

	Male	Female	Combined
LD50(mg/kg)	323.2	402.1	362.7
95% CI	(268.8-360.3)	(362.3-636.4)	(332.2-401.6)

Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
21-AUG-2001 (23)

Type:	LD50
Species:	rat
Strain:	no data
Sex:	no data
Number of Animals:	
Vehicle:	no data
Value:	290 mg/kg bw
Method:	
Year:	GLP: no data
Test substance:	other TS: monoethylaniline; purity not noted
Remark:	When given at one-half its LD50, monoethylaniline caused normochromic anemia and increased by 50-60% the blood methemoglobin content in rats. After chronic administration at 5% the LD50, a decrease in hemoglobin and erythrocytes, and an increase in methemoglobin and leukocytes was observed.

24-APR-2001 (24)

Type:	LD50
Species:	rat
Strain:	
Sex:	
Number of Animals:	
Vehicle:	
Value:	300 mg/kg bw
Method:	other: no data
Year:	GLP: no data
Test substance:	no data

10-AUG-2000 (25)

Type:	LD50
Species:	mouse
Strain:	no data
Sex:	no data
Number of Animals:	
Vehicle:	no data
Value:	500 mg/kg bw
Method:	other: no data
Year:	GLP: no data
Test substance:	other TS: monoethylaniline; purity not noted

24-APR-2001 (24)

Type: LD50
Species: cat
Strain:
Sex:
Number of Animals:
Vehicle:
Value: 25 - 200 mg/kg bw
Method: other: no data
Year: GLP: no data
Test substance: no data
Remark: Report outlines environmental health data from published literature and industry.
Result: No deaths ocurred at 25 mg/kg bw. All animals dies at 200 mg/kg bw.
10-AUG-2000 (16)

5.1.2 Acute Inhalation Toxicity

Type: LC50
Species: rat
Strain:
Sex: male/female
Number of Animals:
Vehicle:
Exposure time: 4 hour(s)
Value: 1.13 - 1.48 mg/l
Method: other: OECD Acute Inhalation Toxicity Protocol - Modified
Year: GLP: yes
Test substance:
Remark: Groups of 5 male and 5 female Sprague Dawley rats (70 total animals) were exposed to chamber concentrations of N-ethylaniline at 0.01, 0.026, 0.30, 1.13, 1.48, 1.38, and 1.42 mg/L. The average particle size (mass median diameter) ranged form 3.8 to 5.8 um (standard deviation of 2.5 to 6.0). Daily observations indicated that body weight loss, nasal discharge, decreased activity, and possible slight respiratory difficulty occurred subsequent to exposure. No lesions definitely attributable to N-ethylaniline exposure were noted during post mortem examination. The LC50 (based on actual chamber concentration) was found to be greater than 1.13 and less than 1.48 mg/L.
Test substance: Commercial purity: 97.5%
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
21-AUG-2001 (26)

5.1.3 Acute Dermal Toxicity

Type:	LD50
Species:	rabbit
Strain:	New Zealand white
Sex:	male/female
Number of Animals:	5
Vehicle:	other: undiluted
Value:	> 2000 mg/kg bw
Method:	other: USEPA TSCA Health Effects Testing Guidelines, 40CFR 798.1100, "Acute Dermal Toxicity"
Year:	1992 GLP: yes
Test substance:	other TS: N-ethylaniline, purity 99.19%
Remark:	5 animals/sex/dose group; Test material analysis not done under GLP
Reliability:	(1) valid without restriction GLP guideline study
Flag:	Critical study for SIDS endpoint

21-AUG-2001 (27)

Type:	LD50
Species:	rat
Strain:	
Sex:	male
Number of Animals:	
Vehicle:	
Value:	= 1915.1 mg/kg bw
Method:	other: OECD Protocol - Modified
Year:	GLP: yes
Test substance:	
Remark:	Six male and 6 female rats were assigned to each of the five dosage groups (1200, 1483, 1833, 2265, and 2800 mg/kg). The clipped test area constituted no less than 10% of the entire body surface and was abraded in 3 males and 3 females per group prior to application. Clinical observations included black urine, loss of appetite, decreased activity and death.
Test substance:	Commercial purity: 97.5%
Reliability:	(1) valid without restriction GLP guideline study
Flag:	Critical study for SIDS endpoint

21-AUG-2001 (28)

Type: LD50
Species: rat
Strain:
Sex: female
Number of Animals:
Vehicle:
Value: = 1347 mg/kg bw
Method: other: OECD Protocol - Modified
Year: GLP: yes
Test substance:
Remark: Six male and 6 female rats were assigned to each of the five dosage groups (1200, 1483, 1833, 2265, and 2800 mg/kg). The clipped test area constituted no less than 10% of the entire body surface and was abraded in 3 males and 3 females per group prior to application. Clinical observations included black urine, loss of appetite, decreased activity and death.
Test substance: Commercial purity: 97.5%
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
21-AUG-2001 (28)

5.1.4 Acute Toxicity, other Routes
-

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation
-

5.2.2 Eye Irritation
-

5.3 Sensitization
-

5.4 Repeated Dose Toxicity

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 106-49-0; 108-44-1; 121-69-7; 91-66-7.

5.5 Genetic Toxicity 'in Vitro'

Type: Bacterial reverse mutation assay
System of testing: S. typhimurium strains TA97, TA98, TA100, and TA1535
Concentration: 0, 10.0, 33.0, 100.0, 333.0, 1000.0, and 1666.0 ug/plate
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year: 1983 GLP: yes
Test substance: other TS: N-Ethylaniline (103-69-5), purity: 97% by label
Remark: Procedure: Preincubation protocol used.
Max. 0.05 ml DMSO solvent used/plate.
Plates/test: 1.
Activation system: 10 and 30% S-9 fraction of Arochlor 1254-induced male Sprague-Dawley rat and Syrian hamster livers.
Media: Histidine dependent (Vogel-Bonner).
Assay was done at SRI International.
Reliability: (1) valid without restriction
GLP guideline study
Flag: Critical study for SIDS endpoint
21-AUG-2001 (29)

Type: Bacterial reverse mutation assay
System of testing: Species/Strain: S. typhimurium TA98, TA100, TA1535, TA1537
Concentration: No Data
Cytotoxic Conc.:
Metabolic activation: with and without
Result: negative
Method: other: similar to OECD Guide-line 471
Year: GLP: yes
Test substance: no data
Remark: Procedure: Pre-incubation.
Plates/test: No data.
Activation system: S-9 liver fraction from Arochlor 1254 or methylcholanthrene induced rats.
Media: histidine dependent.
No. of replicates: No data.
Reliability: (1) valid without restriction
Comparable to Guideline study
Flag: Critical study for SIDS endpoint
21-AUG-2001 (30)

5.6 Genetic Toxicity 'in Vivo'
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5.7 Carcinogenicity

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5.8 Toxicity to Reproduction

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 106-49-0; 108-44-1; 121-69-7.

5.9 Developmental Toxicity/Teratogenicity

See IUCLID data sets on CAS# 62-53-3; 95-53-4; 121-69-7; 91-66-7.

5.10 Other Relevant Information

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5.11 Experience with Human Exposure

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(1) Verschueren, K. (2001) Handbook of Environmental Data on Organic Chemicals, 4th Edition. volume 2. John Wiley & Sons: New York. pps 835-6.

(2) CRC Handbook of Chemistry and Physics. 80th edition (1999-2000) David R. Lide, ed. CRC Press, New York. p 3-23, #743.

(3) Merck Index, 11th Edition, 1989

(4) CRC Handbook of Chemistry and Physics. 80th edition (1999-2000) David R. Lide, ed. CRC Press, New York. p 6-84.

(5) Tonogai, Y. (1982)

(6) Ichikawa Y, Yamano T, Fujishima H. 1969. Biochim. Biophys. Acta. 171:32.

(7) Sangster, J. 1989. J. Phys. Chem. Ref. Data 18(3):1201.

(8) Schultz OE, Jung C. Moeller KE. 1970. Z. Naturforscher B. 25:1024

(9) Meylan W. and Howard P. (1999) EPIWin Modeling Program. Syracuse Research Corporation. Environmental Science Center, 6225 Running Ridge Road, North Syracuse, NY 13212-2510

(10) Zoeteman BCJ, Harmsen K, Linders JBHJ, Morra CFH, Slooff W. (1980). Chemosphere. 9(4):231-49.

(11) Verschueren, K. (2001) Handbook of Environmental Data on Organic Chemicals, 4th Edition. volume 1. John Wiley & Sons: New York. pps 1076.

(12) BASF AG: Unveröffentlichte Untersuchungen des Instituts Kuhlmann, Analysen-Nr. 2-629-33/89a (1988) [unpublished study....], cited in BUA Report Nr. 51 on N-Ethylaniline.

(13) German Chemical Society, July 1990. BASF AG, 1990.

(14) Tonogai, Y., Actual Survey on TLM (Median Tolerance Limit) Values of Environmental Pollutants, Especially of Amines, Nitriles, Aromatic Nitrogen Compounds and Artificial Dyes, Journal Toxicology Science, 7: 193-203, 1982.

(15) Hoechst, AG, Unveroffenlichte Mitteilung, 1982.

(16) German Chemical Society, BUA Report 51, July 1990

(17) Adema DMM, Kuiper J, Hanstveit AO, Canton HH. (1983). Editor(s): Miyamoto J & Kearney PC. Pestic. Chem.: Hum. Welfare Environ., Proc. Int. Congr. Pestic. Chem., 5th Meeting Date 1982. Publisher: Pergamon, Oxford, UK. pps.537-44.

(18) Yoshioka Y, Ose Y, Sato T. SCIENCE OF THE TOTAL ENVIRONMENT (1985, May), 43(1-2):149-57.

(19) Liebmann, H. (1962)

(20) BASF AG: Unveröffentlichte Untersuchungen von Dr. Noack. 1989. Laboratorium for angewandte Biologie, Journal-Nr. 09821.

(21) Batterton J, Winters K, Van Baalen C. Science (1978). 199(4333):1068-70.

(22) ChemFirst Study No. L08684-12

(23) FDRL Study 6771-E. February 18, 1981.

(24) Yalkut, S. I. USSR. Gig. Primen., Toksikol. Pestits. Klin. Otravl. (1971), No. 9 360-2. From: Ref. Zh., Biol. Khim. 1972, Abstr. No. 6F2173. Journal written in Russian.

(25) Dieke, S.H., et al. (1947)

(26) FDRL Report of Study 6771-E, December 17, 1981.

(27) ChemFirst Study No. L08684-13

(28) FDRL Report of Study 6771-E, April 18, 1981.

(29) Zeiger, E. et al (1988) Environ. Mol. Mutagen. Vol. II (Suppl. 12): 1-158.

(30) Florin, I., et al. (1980) Screening of Tobacco Smoke Constituents for Mutagenicity Using the Ames Test. Toxicology, 18:219-232.

7.1 End Point Summary

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7.2 Hazard Summary

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7.3 Risk Assessment

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